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and Space Administration

**Scientific and Technical
Information Branch**

Preface

A mathematical model of the internal combustion engine has been constructed and implemented as a computer program suitable for use on large digital computer systems. The model strikes a balance between three competing factors: (1) the desire for physical realism, (2) the extent of experimental information on the physical processes occurring in the engine, and (3) the capabilities of today's generation of computers. The result is a flexible and computationally economical model based on a system of ordinary differential equations for cylinder-averaged properties. The computer program is capable of multicycle calculations, with some parameters varying from cycle to cycle, and has restart capabilities that permit continuation of a sequence of cycle calculations or the recalculation of earlier cycles with altered assumptions. It can accommodate a broad spectrum of reactants, permits changes in physical properties, and offers a wide selection of alternative modeling functions without any reprogramming. It readily adapts to the amount of information available in a particular case because the model is actually a hierarchy of five models of differing complexity. The models range from a simple model requiring only thermodynamic properties to a very complex one demanding full combustion kinetics, transport properties, and poppet valve flow characteristics. These five models can be defined precisely only by the governing equations. However, they can still be classified approximately according to their treatment of several important features of the internal combustion engine. This classification is shown in the accompanying table, where level 1 represents the simplest model and level 5 the most complex. The calculations are based on the premise that heat transfer is expressible in terms of a heat transfer coefficient and that the cylinder average of kinetic plus potential energies remains constant. Furthermore, during combustion the pressures of the burned and unburned gases are assumed to be equal and their heat transfer areas are assumed to be proportional to their respective mass fractions. Although the model cannot resolve spatial gradients, it does not assume spatial uniformity.

The mathematical model, the numerical techniques, and the associated computer program are all discussed in the four chapters of this report. Chapter I, "Construction of Mathematical Models of the Internal Combustion Engine," briefly summarizes the history of experimental and modeling studies of the internal combustion engine and derives the mathematical model. Chapter II, "Numerical Integration of Ordinary Differential Equations," analyzes the integration techniques used to implement the model. Chapter III, "Numerical Details and Definitions of Cycle Performance Parameters," gives the precise forms of all equations used in the computer program and defines the calculated parameters that are used as measures of cycle performance. It also defines the fresh charge to the engine and gives the representation used for the thermodynamic and transport properties. Chapter IV, "The Organization and Use of Computer Program ZMOTTO," describes program capabilities and input requirements. It presents the results of six sample calculations and briefly describes each computer program routine.

<table>
<tr><th rowspan="2">Feature</th><th colspan="5">Modeling level</th></tr>
<tr><th>5</th><th>4</th><th>3</th><th>2</th><th>1</th></tr>
<tr><td>Flow</td><td colspan="2">Poppet valve formulas</td><td colspan="3">Zero-pressure-drop flow; flow reversal only at $\theta = 0$ or $\theta = 3\pi$, where pressure discontinuities are possible</td></tr>
<tr><td>Flame</td><td>Kinetic</td><td colspan="4">Equilibrium</td></tr>
<tr><td>Flame propagation</td><td colspan="4">Mass burning formulas</td><td>Instantaneous</td></tr>
<tr><td>Burned-gas chemistry</td><td colspan="3">Finite rate</td><td colspan="2">Equilibrium</td></tr>
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Contents

Chapter I

Construction of Mathematical Models of the Internal Combustion Engine

Frank J. Zeleznik

The four-stroke, spark-ignited, internal combustion engine, familiar to almost everyone as the powerplant for the ubiquitous automobile, had its genesis in 1876. It sprang into existence from the work of Nicolaus August Otto, and the history of its birth pangs was recounted by Bryant (ref. 1). The general principle of operation, often referred to as the Otto cycle, has been the object of experimental and theoretical study, at ever increasing levels of sophistication, from that time to the present. The early impetus for the work was the desire to improve engine performance, economy, and reliability. In more recent years these goals have been supplemented by the palpably perceived need to control the emission of pollutants. The four-stroke operation of the engine (a cylinder fitted with a movable piston, separate intake and exhaust systems, and a spark plug for ignition) is simplicity itself when viewed on a sufficiently coarse scale. A schematic representation of its operation is shown in figure 1. A mixture of fuel and air is ingested during the intake stroke, compressed by the piston during the compression stroke, ignited and burned, expanded during the power stroke, and finally exhausted from the cylinder as burned gases during the exhaust stroke in preparation for a repetition of the cycle. Yet this basic simplicity conceals a complexity of interacting physical and chemical processes which has successfully defied complete understanding. The reason for this is easily comprehended when we look a little more closely:

(1) The system is an open one, operating at relatively high temperatures and pressures, which retains a memory of the preceding cycle. The memory arises because the cylinder is not completely evacuated at the end of each cycle and because the end of one cycle provides initial conditions for the following cycle.

(2) The operation has a repetition rate ranging from about 25 to 250 msec.

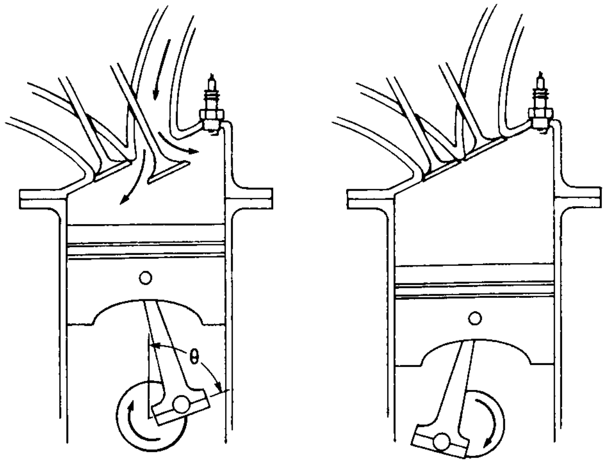
(3) Some very complex chemistry (hydrocarbon combustion) is taking place, and the time scale for some of the chemical reactions is comparable to the cycle repetition rate.

(4) The system has movable boundaries and a complex geometry which seriously complicate the fluid mechanics and heat transfer.

(5) The engine operation is not strictly repeatable because the engine undergoes apparently random cycle-to-cycle variations.

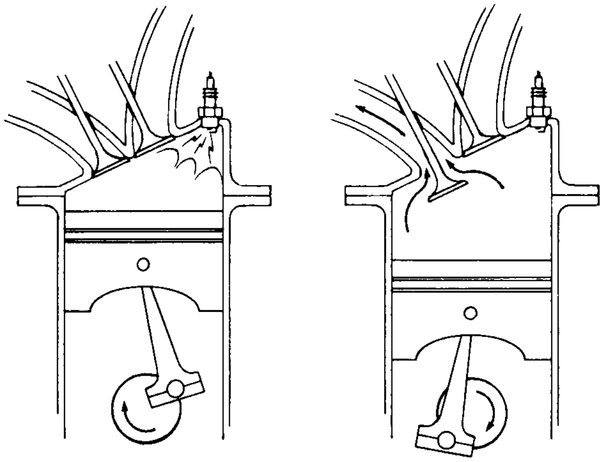
The net result of these five factors is a system that exhibits strong temporal and spatial gradients during a cycle and relatively large fluctuations from one cycle to the next. This situation is inimical to unsophisticated experimentation and simple computation. It requires the ingenious use of novel experimental techniques and modern computational stratagems to achieve even a relatively crude understanding and modeling of this complex system's physical processes.

The extent of our experimentally derived understanding of the physical and chemical processes taking place in the internal combustion engine can be gleaned from some fairly recent survey papers (refs. 2 to 5). The intake and exhaust portions of the cycle generate highly turbulent flows within the cylinder (ref. 5, p. 145) and the ignition-combustion process is influenced by the level of turbulence (ref. 2, p. 131, and ref. 5, p. 156). Ignition of the combustible mixture produces a propagating flame



(a) Intake stroke, $0 \leq \theta \leq \pi$.

(b) Compression stroke, $\pi \leq \theta \leq 2\pi$.



(c) Power stroke, $2\pi \leq \theta \leq 3\pi$.

(d) Exhaust stroke, $3\pi \leq \theta \leq 4\pi$.

Figure 1. - Four-stroke operation of spark-ignited internal combustion engine.

front, whose shape deviates appreciably from sphericity, and chemical reactions continue after the passage of the flame front (ref. 2, p. 121, fig. 2). Some attractive color photographs of the flame front, its propagation, and the postflame reaction zone are presented by Nakanishi et al. (ref. 6). There is also some evidence for the existence of preflame chemical reactions in the combustible mixture (ref. 2, p. 123). The chemical reactions in the flame front and the postflame and preflame chemical reactions are quenched near cool walls and in crevices; the quenching effect extends out from the surface as much as 0.4 mm (ref. 2, pp. 124 to 126, figs. 8 and 9). Temperature gradients (ref. 2, p. 120) and composition gradients (ref. 4, p. 140, fig. 6) occur throughout the cylinder and not just near the walls. More than 200 organic compounds (ref. 4, p. 143) have been identified in the exhaust gases by gas chromatography (ref. 3, p. 163, fig. 9). Finally the nitric oxide concentration in the exhaust gases seems to depend on its rate of formation as well as its rate of decomposition within the engine (ref. 2, p. 128).

These experimental conclusions are undoubtedly correct, but in many instances they represent only qualitative results from poorly controlled experiments. One reason for this situation is the unfortunate coupling between an inability to achieve cycle-to-cycle repeatability in the operation of the engine and an inability to measure a single cycle adequately. For example, Starkman et al. (ref. 7) carried out a sampling study of the burned gases in an engine cylinder by withdrawing a small sample from many successive cycles. Thus their conclusions represent cycle-averaged results. They observed (1) that wall quenching affects carbon monoxide, carbon dioxide, and nitric oxide formation as much as it affects unburned hydrocarbons and (2) that large composition gradients exist within the cylinder. Similarly, in a spectroscopic investigation of nitric oxide formation, Lavoie et al. (refs. 8 and 9) obtained cycle-averaged results. They sampled only from those cycles whose peak pressures were within a certain interval (nearly 3 atm, ref. 9) about a preselected pressure. From their results they concluded that substantial temperature and nitric oxide concentration gradients exist behind the flame front (ref. 9, p. 107). The existence of gradients and their dependence on engine geometry make experimental results a function of the measurement locale. Consequently comparisons of experimental results from various investigators are virtually impossible because of differences in engine geometry, measurement location, and measurement technique. Even if these three difficulties were surmounted, comparisons would still be thwarted by cycle-to-cycle variations.

Since steep temporal and spatial gradients are acknowledged conditions in internal combustion engines, what are the prospects for obtaining quantitative experimental results capable of resolving these gradients within an engine? The prospects are decidedly dismal. The capability to carry out spatially resolved measurements is limited by the presence of moving valves and pistons, which drastically restrict the positioning of probes within an engine. Furthermore the hostile environment places severe limitations on the types of probes which can be used. For example, hot-wire turbulence measurements have only been made on motored engines, where combustion is not a factor (ref. 5, p. 146). Optical diagnostic techniques now in the process of development offer some advantages over probes, but they too are no panacea (refs. 10 to 14). Under the present circumstances even an optimist would find it difficult to imagine that spatially and temporally resolved measurements adequate to unravel the complex of physical and chemical processes taking place in an engine would become available in the near future.

Serious attempts to construct models of the internal combustion engine began about 1960. It was at this time that digital computers were becoming increasingly available and more capable. Before that time calculations were largely done by hand or were done with the assistance of mechanical calculators. This severely limited the kinds of computations which could be attempted. Since then the numerical models have increased in number and complexity. A representative sampling of computer-oriented models of the internal combustion engine is listed in nearly chronological order in table I, where the models (refs. 15 to 39) are broadly classified by the choice of equations and the treatment of chemistry, combustion, heat transfer, working fluid induction, working fluid exhaust, and valve timing. This classification is only suggestive rather than definitive for often there is great variability in the treatment of a particular aspect among the models. Thus two models might both consider chemical kinetics—one with a relatively detailed mechanism, the other with a drastically truncated one—yet both can be thought of as treating the chemistry kinetically. Models with identical classifications in table I can, and generally will, differ considerably in the treatment of physical and chemical properties, in the modeling of physical processes, and in the numerical and analytical details of the calculation. Consequently they will also differ to a greater or lesser degree in the answers they supply. Because of this fine structure it would be pointless to attempt a more detailed comparison of these models, but one general observation is in order. Most of these models give short shrift to the chemical and physical properties of the working fluid. This is unfortunate because then one cannot be certain how much of a model's deficiency is ascribable to inadequate working fluid properties and how much must be assigned to the other details of the model.

Structure of a Realistic Model

The numerical realization of a mathematical model for a physical system, in the form of a computer program, is shaped by a combination of practical and philosophical decisions which determine its ultimate form. These decisions reflect the modeler's perception of what is necessary, desirable, and achievable. The choice between ordinary differential equations or partial differential equations represents such a decision. A computer program for modeling is composed of two essential but independent parts: (1) the set of equations used to model the physical system and (2) the data base of physical and chemical properties used in the implementation of those equations. They, in concert with numerical techniques, determine the results of model calculations. But estimates of physical properties are obtained, revised, and improved independently of any changes in the model itself.

TABLE I. - REPRESENTATIVE SAMPLING OF COMPUTER MODELS OF INTERNAL COMBUSTION ENGINE

	Chemistry		Combustion		Wall heat trans-fer	Working fluid induc-tion	Working fluid exhaust	Valve timing	Differential equations			
	Thermo-dynamic	Kinetic	Instan-taneous	Burn-ing rate					Ordi-nary	Partial		
										Par-tial	Space vari-ables	Grid
N. D. Whitehouse et al. (ref. 15)				✓	✓	✓	✓	✓	✓			
M. H. Edson (ref. 16)	✓		✓			✓	✓					
D. J. Patterson and G. Van Wylen (ref. 17)	✓			✓	✓	✓	✓		✓			
F. M. Strange (ref. 18)	✓			✓	✓	✓	✓		✓			
K. J. McAulay et al. (ref. 20)				✓	✓	✓	✓	✓	✓			
P. Huber and J. R. Brown (ref. 19)				✓	✓	✓	✓	✓	✓			
W. J. D. Annand (ref. 21)	✓	✓		✓	✓				✓			
J. B. Heywood et al. (refs. 8 and 22) and P. Blumberg and J. T. Kummer (ref. 23)	✓	✓		✓					✓			
L. J. Spadaccini and W. Chinitz (ref. 24)	✓	✓	✓		✓				✓			
G. G. Lucas and E. H. James (ref. 25)	✓			✓	✓				✓			
S. Srivatsa (ref. 26)	✓	✓		✓	✓				✓			
H. Hiroyasu and T. Kadota (ref. 27)	✓	✓		✓	✓				✓			
L. D. Browning and R. K. Pefley (ref. 28)		✓		✓	✓	✓			✓			
S. D. Hires et al. (ref. 29)	✓	✓		✓	✓	✓	✓	✓	✓			
J. J. Fagelson et al. (ref. 30)	✓	✓		✓					✓			
W. A. Sirignano (ref. 31)				✓						✓	1	?
J. R. Bellan and W. A. Sirignano (ref. 32)	✓	✓		✓	✓					✓	1	?
F. V. Bracco and W. A. Sirignano (ref. 33)				✓	✓					✓	1	?
A. A. Boni, M. Chapman, and G. P. Schneyer (refs. 34, 35)	✓	✓		✓						✓	1	50
A. A. Boni, M. Chapman, and G. P. Schneyer (refs. 35, 36)	✓	✓		✓						✓	2	10x25
M. D. Griffin et al. (ref. 37)			✓			✓	✓			✓	2	10x9
M. D. Griffin et al. (ref. 38)			✓			✓	✓			✓	3	7x9x10 + 10 or 10x9x9
M. D. Griffin et al. (ref. 38)		✓		✓		✓	✓			✓	2	10x9
A. D. Gosman and A. P. Watkins (ref. 39)					✓	✓	✓			✓	2	21x21

Hence a computer program should be so constructed that it is a relatively simple task to incorporate additional or improved property data as they become available. Ideally the best and most complete data base should be used in the calculations. This approach permits the modeler to stop worrying about the effect of unnecessary data assumptions on the calculation and to concentrate on the model itself. All too often apparently insignificant data changes produce unexpectedly large effects on the calculated results.

It is axiomatic that the more detailed the model, the more complex the calculation and the more difficult the specification of that model. Thus, for example, a calculation which ignores heat loss is simpler and requires less information than one which considers heat transfer, for we must know, estimate, or assume the heat transfer rates. Increasing the complexity of the model does not necessarily increase the validity of the results although it certainly has the potential for doing so. The utility and validity of the results from a model calculation are only as good as the information used to construct the model and the user's understanding of the inherent limitations, both physical and numerical, of the model.

A given level of model complexity may sometimes require more information than is available in a particular situation. Under these circumstances it is an advantage to have simpler models which need less information to define the calculation. Thus it seems reasonable to construct a hierarchy of models differing in complexity. A second advantage of such a hierarchy is the possibility of comparing results among the hierarchy and thus judging the significance of simplifying assumptions.

What are the prospects for a realistic modeling of the internal combustion engine? There is no absolute answer to this question for it is an ambiguous one. All too often realism, like beauty, is in the eye of the beholder and mirrors his own interests as much as reality. This is particularly true when experimental information is incomplete and computational capabilities are inadequate for a complete solution of the problem, as is the case with the internal combustion engine. My own brand of realism leads me to conclude that a computer model must be capable of multicycle calculations so that it can converge to the conditions that exist during the steady state operation of the engine and so that it can look at cycle-to-cycle variations in the operation of the engine. It must account for heat transfer at the walls because heat losses represent approximately a third of the energy liberated by combustion. These losses strongly affect the temperature of the working fluid, which in turn has a strong effect on the rate processes taking place in the working fluid. It must be capable of representing the valve timing of the intake and exhaust systems since this influences the amount and composition of both the working fluid and the exhaust gases. It must permit a fully kinetic treatment of the chemistry rather than just a truncated reaction mechanism supplemented by steady state assumptions. Steady state assumptions can only be justified *a posteriori*, that is, by a comparison with results from a fully kinetic treatment. These characteristics I believe to be the indispensable components of a realistic model.

What are the implications of the experimental and computational state of affairs for modeling the internal combustion engine at this level of realism? There are some who would perhaps argue that the presence of spatial gradients is *prima facie* evidence that modeling with a system of partial differential equations is necessary and anything less is unrealistic. However, this brand of realism would require the solution of a system of partial differential equations in time and three spatial coordinates because typical engines lack any spatial symmetry in their configurations. Since meaningful modeling of the internal combustion engine cannot ignore the chemistry involved, this portends a very large system of partial differential equations. These must be solved numerically on a space and time grid which is adequate for resolving the spatial and temporal gradients, and they must be solved for a number of consecutive cycles. Just as there are yet no adequate experimental data to validate the results of such a detailed computation, so too there are no adequate data to supply the necessary initial and boundary values for this computation. These values must then be obtained by assumption. But, as anyone who has ever solved a differential equation will realize, the character of a solution can depend on these subsidiary conditions as strongly as on the differential equation. The assumed conditions thus naturally diminish the reality of the calculated results. Furthermore the full-blown problem is such an awesome numerical task, incapable of realization with the present generation of computers and algorithms, that one must also resort to very coarse grids and some drastic simplifying assumptions for purely numerical and economic reasons. All of these factors conspire to eliminate partial differential equations as a vehicle for realistic modeling. Exact calculations of this type are not now feasible nor will they soon be. Consequently the modeling must be accomplished with a system of ordinary differential equations. The restriction to ordinary differential equations is not a serious one for, as will be shown, it is possible to derive a system of ordinary differential equations without invoking an assumption of spatial homogeneity. Thus, although ordinary differential equations cannot be used to resolve spatial gradients, they are valid in their presence.

A simple commitment to ordinary differential equations does not by itself resolve all questions concerning the modeling of internal combustion engines. The meager and problematical experimental data portend an uncertainty in the selection of a definitive system of differential equations. The best one can reasonably expect is to construct a parametric system of differential equations whose solutions cover the gamut of observed behavior. The parameters, one hopes, can then be determined by a comparison of calculated results with experimental measurements. But there is a caveat. It is most likely that the solutions will be nonlinearly dependent on the parameters, and so it would not be surprising if a unique set of parameters could not be obtained even with the availability of precise and accurate experimental measurements. Nonetheless that is the approach I shall follow.

This part of the report describes the mathematical and physical aspects of a hierarchy of models for the internal combustion engine. The discussion includes the derivation of the governing differential equations, the specification of the forms for the modeling functions which they contain, and the treatment of the physical and chemical properties used in the solution of the differential equations. These fundamental features of the model combine to determine its basic validity, and their comprehension is essential for an understanding of the results obtained from the model. A description of a preliminary version of the model was given in 1977 (ref. 40).

Mathematical Model

Derivation of General Differential Equations

The internal combustion engine shares with other technologically important physical systems the characteristics of spatial and temporal gradients and many chemically transforming species. Such reacting systems occur not only in the internal combustion engine but also in other combustion-based vehicle powerplants, in reactors for the chemical industry, in industrial furnaces, in stationary powerplants, and in the context of environmental and atmospheric problems. The analytical solution of the large system of partial differential equations characterizing such physical systems is impossible; the numerical solution is impractical. Sheer pragmatism forces us to describe the physical system by a collection of ordinary differential equations. The systems of ordinary differential equations fall into one of two categories. One type describes the transient behavior of a nonflowing physical system. The other characterizes the steady state behavior of a flowing system. These equations are conventionally obtained from the corresponding partial differential equations by imposing simplifying assumptions and neglecting dissipative and transport phenomena. The equations for transient behavior result from the assumption of spatial uniformity. The steady state equations are obtained by assuming that temporal derivatives vanish and that spatial derivatives vanish in two of three coordinate directions. But clearly the physical systems which one would like to analyze generally do not satisfy these criteria, and it would be comforting to work with equations which do not rely on such strong assumptions. I shall derive appropriate systems of equations for each of the two categories without any assumptions about constitutive relations, dissipation, or vanishing derivatives, but it will be necessary to reinterpret the dependent variables. This procedure significantly enlarges the number of physical systems which can be justifiably modeled with ordinary differential equations. The derivation will not be directed specifically toward the internal combustion engine but will be done more generally because the resulting equations are equally applicable to other systems. It is only the choice of modeling functions which makes the equations specific for a particular physical system.

The derivation will be based on a system of partial differential equations describing the evolution of the dependent variables. These equations can be written most conveniently in the notation of general tensor analysis. I shall employ the convention that Latin indices ($i, j, k, \ldots$) will be tensor indices with the range 1, 2, 3 corresponding to the three-dimensional space of our experience. Greek indices from the first part of the alphabet (α, β, γ, . . .) will have the range 1, 2 and will indicate tensor behavior with respect to transformations of the intrinsic coordinates of some two-dimensional subspace. Greek indices from the last part of the alphabet will be nontensor indices. When they are unbarred (λ, μ, ν, . . .), they will be used to enumerate the different chemical species and hence will have an indefinite range which becomes definite in any given application. When they are barred ($\bar{\lambda}$, $\bar{\mu}$, $\bar{\nu}$, . . .), they will be used to label surfaces which partition the bounding surface of a volume, and they will also have an indefinite range which need not coincide with the range of the unbarred indices. The summation convention on an index repeated as a raised *and* lowered index will apply to all indices whether Latin or Greek, tensor or nontensor, unless an explicit statement to the contrary is made.

The state of a fluid is characterized by two thermodynamic variables, say the mass density m and the internal energy per unit mass u, and by composition variables per unit mass n_λ. This assumes that electromagnetic effects are negligible. The evolution equations for these variables and the kinetic energy are (ref. 41)

$$\frac{\partial(mu)}{\partial t} + \nabla_k(muv^k) = -\nabla_k(q^k + \hat{\mu}^\lambda d^k_\lambda) + \tau^{kj}\nabla_j v_k - m\frac{\partial\Omega}{\partial t} - v^k f_k = m\frac{\delta u}{\delta t} \tag{I-1}$$

$$\frac{\partial m}{\partial t} + \nabla_k(mv^k) = 0 = \frac{\delta m}{\delta t} + m\nabla_k v^k \tag{I-2}$$

$$\frac{\partial(mn_\lambda)}{\partial t} + \nabla_k(mn_\lambda v^k + d^k_\lambda) = R_\lambda \tag{I-3}$$

$$\frac{\partial[m(v^i v_i/2 + \Omega)]}{\partial t} + \nabla_k\left[m\left(\frac{v^i v_i}{2} + \Omega\right)v^k - \tau^{ik}v_i\right] = -\tau^{kj}\nabla_j v_k + m\frac{\partial\Omega}{\partial t} + v^k f_k \tag{I-4}$$

In these equations v^k is the fluid velocity, q^k is the heat flux, $\hat{\mu}^\lambda$ is the internal energy transported by diffusion of one mole of species λ, d^k_λ is the diffusive flux of the species λ, τ^{kj} is the stress tensor, Ω is the potential energy, f_k represents all volumetric forces over and above those produced by the stress τ^{kj} and the potential Ω, while R_λ is the volumetric rate of production of species λ. The symbol t is the time, ∇_k is the covariant derivative with respect to the coordinates of the three space, and $\delta/\delta t = \partial/\partial t + v^k\nabla_k$ is variously known as the absolute, substantial, or convective derivative. These equations are predicated upon writing the evolution equation for the velocity in the form

$$m\frac{\delta v^k}{\delta t} = F^k = -mg^{ki}\nabla_i\Omega + f^k + \nabla_j\tau^{kj} \tag{I-5}$$

where g^{ki} are the contravariant components of the metric tensor whose covariant components are g_{ij}. We need not be concerned with the forms of the constitutive relations for q^k, $\hat{\mu}^\lambda$, d^k_λ, Ω, f_k, and R_λ since they are irrelevant to the present calculation. However, it will be convenient to decompose the stress tensor into two parts.

$$\tau^{kj} = -pg^{kj} + \Delta\tau^{kj} \tag{I-5a}$$

The first term on the right represents the contribution of pressure p to the stress, while $\Delta\tau^{kj}$ may be regarded as the dissipative stresses. Once more, the form of p and $\Delta\tau^{kj}$ will be of no concern to us. This decomposition of the stress enables us to obtain an evolution equation for the enthalpy per unit mass, $h = u + p/m$, which is sometimes used in place of the internal energy. The equation for h can be obtained from the equation for u if we can deduce an equation for p/m. This is easily done by invoking the continuity equation (I-2).

$$-pg^{kj}\nabla_j v_k = -p\nabla_k v^k = \frac{p}{m}\ \frac{\delta m}{\delta t} = -m\frac{\delta(p/m)}{\delta t} + \frac{\delta p}{\delta t}$$

If this result is used, then the equation for *h* is

$$\frac{\partial(mh)}{\partial t} + \nabla_k(mhv^k) = -\ \nabla_k\left(q^k + \hat{\mu}^\lambda d^k_\lambda\right) + \Delta\tau^{kj}\nabla_j v_k - m\frac{\partial\Omega}{\partial t} - v^k f_k + \frac{\delta p}{\delta t} = m\frac{\delta h}{\delta t} \tag{I-6}$$

These partial differential equations will be used to determine two sets of ordinary differential equations governing the behavior of the mean values of properties where the mean values are defined as averages over a suitable region of space. The generalization of the transient equations will emerge from a look at the temporal evolution of averages over some volume of the three-dimensional space which is enclosed by a surface. The generalization of the steady state equations will arise in connection with the evolution of surface-averaged properties. In both cases it will be necessary to rely on generalizations of Leibnitz's rule for the differentiation of an integral with variable limits. Suppose that x^k are coordinates covering the space and that $\varphi = \varphi(x^k, t)$ is a scalar density which is to be integrated over a volume V enclosed by the surface A (fig. 2). Both the surface and the volume may be functions of time. Then the generalization of the Leibnitz rule to three dimensions is

$$\frac{d}{dt}\int_{V(t)}\varphi\, dv = \int_{V(t)}\frac{\partial\varphi}{\partial t}\,dv + \int_{A(t)}\varphi V^i n_i\, da \tag{I-7}$$

where dv is the element of volume, da is the element of area, n_i is the exterior normal to $A(t)$, and V^i is the velocity of a point on the surface. Although several physical quantities have been mnemonically designated by the 22nd letter of the alphabet, no confusion should occur because V and V^i differ by the absence or presence of an index as do v and v^i. Furthermore, for the sake of convenience, let me introduce the conventional notation $v^2 = v^k v_k$. Note that the integral on the left side of equation (I-7) is only a function of t since the coordinate dependence has been integrated out and hence the notation d/dt is correct. The integral relation (I-7) is the indispensable tool which will be used to derive the generalized ordinary differential equations for transient behavior. If we set φ equal to 1 in equation (I-7), then we get as a special case

$$\frac{dV}{dt} = \int_{A(t)} V^i n_i\, da \tag{I-8}$$

The case of surface averages is somewhat more difficult to describe. Basically the system of interest can be thought of as the contents of a tube generated by the propagation of a surface, bounded by a closed curve, through space. For example, the propagation of a circle perpendicular to its plane will generate a cylinder. To describe a more general situation, imagine a one-parameter family of propagating surfaces, $\phi = \phi(x^k, t)$, with each member of the family labeled by the value of ϕ. Of

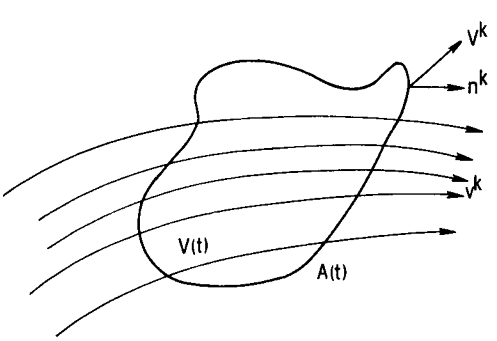


Figure 2. - Sketch of system used in derivation of transient equations.

course the function $\phi(x^k, t)$ might be independent of t. Suppose that on each surface we inscribe a closed curve C which bounds an area A (fig. 3). Both the curve and its enclosed area are potentially functions of t and of the parameter ϕ labeling the surface. The shape of the tube generated in this way may be a function of time. Suppose V^α and W^α are both two-dimensional vectors in the subspace defined by the surface ϕ and represent the rate of change of the closed curve C with respect to t and ϕ, respectively. The vector V^α, for example, can be interpreted as the velocity of a point on the curve. The Leibnitz rule applied to the integral of $\varphi(x^k, t)$ over the surface A in the subspace becomes

$$\frac{\partial}{\partial t}\int_{A(\phi,t)} \varphi\, da = \int_{A(\phi,t)} \frac{\partial \varphi}{\partial t}\, da + \int_{C(\phi,t)} \varphi V^\alpha \eta_\alpha\, dc \tag{I-9}$$

$$\frac{\partial}{\partial \phi}\int_{A(\phi,t)} \varphi\, da = \int_{A(\phi,t)} \frac{\partial \varphi}{\partial \phi}\, da + \int_{C(\phi,t)} \varphi W^\alpha \eta_\alpha\, dc \tag{I-10}$$

The exterior normal to C on the surface ϕ is η_α, dc is an element of arc along C, and again da is an element of area. Analogously to the special case of equation (I-7) represented by equation (I-8) we can obtain special cases of equations (I-9) and (I-10) by choosing $\varphi = 1$.

$$\frac{\partial A}{\partial t} = \int_{C(\phi,t)} V^\alpha \eta_\alpha\, dc \tag{I-11}$$

$$\frac{\partial A}{\partial \phi} = \int_{C(\phi,t)} W^\alpha \eta_\alpha\, dc \tag{I-12}$$

The integral relations (I-9) and (I-10) are the key to the steady state equations.

General transient equations. – To simplify the derivation of the transient equations, we make the preliminary observation that equations (I-1) to (I-4) and (I-6) are similar to one another in the sense that they can all be written in the form of a conservation equation.

$$\frac{\partial (m\psi)}{\partial t} + \nabla_k (m\psi v^k) = S \tag{I-13}$$

Here ψ represents some property per unit mass and S is its volumetric source. Suppose we define a mass-averaged value of ψ for the system of figure 1 by

$$\langle \psi \rangle \equiv \frac{1}{M}\int_{V(t)} m\psi\, dv \tag{I-14}$$

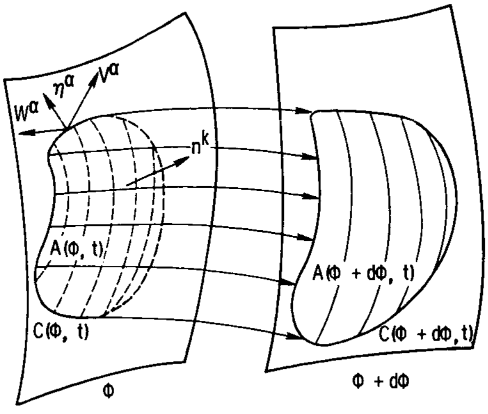


Figure 3. - Sketch of system used in derivation of steady-state equations.

where

$$M(t) \equiv \int_{V(t)} m\, dv \tag{I-15}$$

Differentiation of equation (I-14) with respect to t and the application of the Leibnitz formula (I-7) with $\varphi = m\psi$ gives

$$\frac{d\langle\psi\rangle}{dt} = \frac{1}{M}\left[\int_{V(t)} \frac{\partial(m\psi)}{\partial t}\, dv + \int_{A(t)} m\psi V^k n_k\, da\right] - \frac{1}{M}\frac{dM}{dt}\langle\psi\rangle$$

Equation (I-13) can now be used to rewrite the first integral, and the divergence portion of the resulting volume integral can be converted to a surface integral by Green's theorem.

$$\int_{V(t)} \nabla_k(m\psi v^k) dv = \int_{A(t)} m\psi v^k n_k\, da$$

The result is the expression

$$\frac{d\langle\psi\rangle}{dt} = \frac{1}{M}\int_{V(t)} S\, dv + \frac{1}{M}\int_{A(t)} m\psi(V^k - v^k) n_k\, da - \frac{1}{M}\frac{dM}{dt}\langle\psi\rangle \tag{I-16}$$

A special case of this formula can be obtained by setting ψ equal to 1 in equations (I-14) and (I-16). But then from equation (2) it follows that $S = 0$, and from equations (I-14) and (I-15) we find that $\langle 1 \rangle = 1$. Hence equation (I-16) reduces to

$$\frac{dM}{dt} = \int_{A(t)} m(V^k - v^k) n_k\, da \tag{I-17}$$

Recall that V^k is the velocity of the surface $A(t)$ and that v^k is the fluid velocity. Thus $V^k - v^k$ is the velocity of the surface relative to the fluid. If we define an average density for the volume V by

$$\rho \equiv \frac{M}{V} = V^{-1}\int_{V(t)} m\, dv \tag{I-18}$$

then by direct differentiation we obtain

$$\frac{1}{\rho}\frac{d\rho}{dt} = \frac{1}{M}\frac{dM}{dt} - \frac{1}{V}\frac{dV}{dt} \tag{I-19}$$

Obviously formula (I-16) can be applied to the problem at hand by letting ψ successively become u, h, n_λ, and $\Theta \equiv v^2/2 + \Omega$; the corresponding expressions for S are obtained from equations (I-1), (I-6), (I-3), and (I-4). If all divergence terms in the volume integral of S are converted to surface integrals by Green's theorem, then we obtain the following formulas:

$$\frac{d\langle u\rangle}{dt} = \frac{1}{M}\int_{A(t)} [mh(V^k - v^k) - pV^k n_k] da - \frac{\dot{Q}}{M} - \frac{1}{M}\frac{dM}{dt}\langle u\rangle \tag{I-20}$$

$$\frac{d\langle h\rangle}{dt} = \frac{1}{M}\int_{A(t)} mh(V^k - v^k) n_k\, da - \frac{\dot{Q}}{M} + \frac{\dot{H}}{M} - \frac{1}{M}\frac{dM}{dt}\langle h\rangle \tag{I-21}$$

$$\frac{d\langle n_\lambda\rangle}{dt} = \langle R_\lambda/m\rangle + \frac{1}{M}\int_{A(t)} mn_\lambda(V^k - v^k)n_k\,da - \frac{\dot{N}_\lambda}{M} - \frac{1}{M}\frac{dM}{dt}\langle n_\lambda\rangle \tag{I-22}$$

$$\frac{d\langle \Theta\rangle}{dt} = \frac{1}{M}\int_{A(t)} m\Theta(V^k - v^k)n_k\,da + \frac{\dot{Q}}{M} + \frac{\dot{K}}{M} - \frac{1}{M}\frac{dM}{dt}\langle \Theta\rangle \tag{I-23}$$

where the functions of time $Q(t)$, $H(t)$, $N(t)$, and $K(t)$ are defined by

$$\frac{dQ}{dt} = \dot{Q}(t) \equiv \int_{A(t)} (q^k + \hat{\mu}^\lambda d_\lambda^k)n_k\,da - \int_{V(t)} \left[\Delta\tau^{kj}\nabla_j v_k - \frac{\partial\Omega}{\partial t} + v^k(\nabla_k p - f_k)\right]dv \tag{I-24}$$

$$\frac{dH}{dt} = \dot{H}(t) \equiv \int_{V(t)} \frac{\partial p}{\partial t}\,dv \tag{I-25}$$

$$\frac{dN_\lambda}{dt} = \dot{N}_\lambda(t) \equiv \int_{A(t)} d_\lambda^k n_k\,da \tag{I-26}$$

$$\frac{dK}{dt} = \dot{K}(t) \equiv \int_{A(t)} [v_i\Delta\tau^{ik} - (q^k + \hat{\mu}^\lambda d_\lambda^k)]n_k\,da \tag{I-27}$$

No assumptions have been made to this point and equations (I-20) to (I-23) are exact consequences of the partial differential equations. It is only at this stage that some assumptions must be made. I shall assume that there exists a partitioning of the bounding surface $A(t)$ into surfaces $A_{\bar{\mu}}(t)$ whose union is $A(t)$ and such that on each of these surfaces

$$\frac{dV^{\bar{\mu}}}{dt} \equiv \int_{A_{\bar{\mu}}(t)} V^k n_k\,da = 0 \qquad \text{if and only if} \quad \int_{A_{\bar{\mu}}(t)} pV^k n_k\,da = 0 \tag{I-28}$$

$$\frac{dM^{\bar{\mu}}}{dt} \equiv \int_{A_{\bar{\mu}}(t)} m(V^k - v^k)n_k\,da = 0 \qquad \text{if and only if} \quad \int_{A_{\bar{\mu}}(t)} m\psi(V^k - v^k)n_k\,da = 0 \tag{I-29}$$

for $\psi = u, h, n_\lambda, v^2/2$, and Ω. These assumptions are obviously satisfied when p and ψ are constant on $A_{\bar{\mu}}(t)$. The assumptions (I-28) and (I-29) enable us to define a "volume flux average" of the pressure by

$$p^*_{\bar{\mu}}\,\frac{dV^{\bar{\mu}}}{dt} \equiv \int_{A_{\bar{\mu}}(t)} pV^k n_k\,da \qquad (\bar{\mu}\text{ not summed}) \tag{I-30}$$

where $p^*_{\bar{\mu}}$ denotes the average of the pressure and a "mass flux average" of the scalar field per unit mass ψ by

$$\tilde{\psi}_{\bar{\mu}}\,\frac{dM^{\bar{\mu}}}{dt} \equiv \int_{A_{\bar{\mu}}(t)} m\psi(V^k - v^k)n_k da \qquad (\bar{\mu}\text{ not summed}) \tag{I-31}$$

where $\tilde{\psi}_{\bar{\mu}}$ denotes the average of the scalar ψ. The significance of the functions $\tilde{\psi}_{\bar{\mu}}$ and $p^*_{\bar{\mu}}$ will be discussed shortly; however, it should be pointed out that the partitioning of $A(t)$ used in the definition of $\tilde{\psi}_{\bar{\mu}}$ and that used for $p^*_{\bar{\mu}}$ need not be the same. This was done here only for notational convenience. Combining these definitions with equations (I–20) to (I–23) gives

$$\frac{d\langle u\rangle}{dt} = \frac{1}{M}\left[-p^*_{\bar{\mu}}\frac{dV^{\bar{\mu}}}{dt} + \tilde{h}_{\bar{\mu}}\frac{dM^{\bar{\mu}}}{dt} - \langle u\rangle\frac{dM}{dt} - \dot{Q}(t)\right] \tag{I–32}$$

$$\frac{d\langle h\rangle}{dt} = \frac{1}{M}\left[\tilde{h}_{\bar{\mu}}\frac{dM^{\bar{\mu}}}{dt} - \langle h\rangle\frac{dM}{dt} - \dot{Q}(t) + \dot{H}(t)\right] \tag{I–33}$$

$$\frac{d\langle n_\lambda\rangle}{dt} = \frac{1}{\rho}\left[V(t)^{-1}\int_{V(t)} R_\lambda\, dv\right] + \frac{1}{M}\left[\tilde{n}_{\lambda_{\bar{\mu}}}\frac{dM^{\bar{\mu}}}{dt} - \langle \mathrm{n}_\lambda\rangle\frac{dM}{dt} - \dot{N}_\lambda(t)\right] \tag{I–34}$$

$$\frac{d\langle \Theta\rangle}{dt} = \frac{1}{M}\left[\tilde{\Theta}_{\bar{\mu}}\frac{dM^{\bar{\mu}}}{dt} - \langle \Theta\rangle\frac{dM}{dt} + \dot{Q}(t) + \dot{K}(t)\right] \tag{I–35}$$

From the definitions of $dV^{\bar{\mu}}/dt$ and $dM^{\bar{\mu}}/dt$ it is clear that $dV/dt = \sum_{\bar{\mu}} dV^{\bar{\mu}}/dt$ and $dM/dt = \sum_{\bar{\mu}} dM^{\bar{\mu}}/dt$.

Inspection of equations (I–32) to (I–35) and (I–19) discloses that they are the ordinary differential equations we have been seeking. Virtually all the terms on the right side of these equations are at our disposal for modeling purposes. This certainly applies to the modeling functions $\dot{Q}$, $\dot{H}$, $\dot{N}$, and $\dot{K}$, whose interpretations are obvious from their definitions (eqs. (I–24) to (I–27)). Thus $\dot{Q}$ might be called the net rate of internal energy loss from $V(t)$ since the surface integral represents the rate of loss of internal energy through the surface $A(t)$ by diffusive processes while the volume integral represents the rate of gain of internal energy due to dissipative effects. The interpretations of $\dot{H}$ and $\dot{N}$ are obvious. The function $\dot{K}$ can be given an interpretation in terms of an energy flux. The vector $q^k + \mu^\lambda d^k_\lambda - v_j \Delta\tau^{jk}$ is the energy flux due to heat conduction, mass diffusion, and dissipative stresses. Hence $\dot{K}$ represents the energy addition to the contents of V by these phenomena. The significance of the modeling functions dM/dt and dV/dt has already been explained; $dM^{\bar{\mu}}/dt$ and $dV^{\bar{\mu}}/dt$ have similar interpretations. The term $\rho^{-1}V^{-1}\int_V R_\lambda\, dv$ in equation (I–34) is the rate of production of $\langle n_\lambda\rangle$ and is a product of the reciprocal density and the volumetric average of the local production rate for species λ. The functions $\tilde{\psi}_{\bar{\mu}}$ and $p^*_{\bar{\mu}}$ still need comment. The right side of equation (I–31) represents the rate at which the property ψ is added to the contents of V by flux through the surface $A_{\bar{\mu}}(t)$ (compare with eq. (I–17)). Because ψ is a property of the fluid and because the fluid properties will most likely be different on opposite sides of $A(t)$, it is reasonable to allow $\tilde{\psi}_{\bar{\mu}}$ to have a form dependent on the sign of $dM^{\bar{\mu}}/dt$. Furthermore, since $\langle\psi\rangle$ is the average value of ψ within $V(t)$, it is also reasonable to assume that $\tilde{\psi}_{\bar{\mu}}$ coincides with $\langle\psi\rangle$ when $dM^{\bar{\mu}}/dt$ is negative. Hence we make the assumption

$$\tilde{\psi}_{\bar{\mu}} = \begin{cases} \psi^{(+)}_{\bar{\mu}}(t) & dM^{\bar{\mu}}/dt > 0 \\ \psi^{(-)}_{\bar{\mu}}(t) = \langle\psi\rangle & dM^{\bar{\mu}}/dt < 0 \end{cases} \tag{I–36}$$

This specification of the modeling function $\psi_{\bar{\mu}}$ is called an assumption, even though $\psi^{(+)}_{\bar{\mu}}$ remains completely arbitrary, because it represents a definite and conscious choice for $\psi^{(-)}_{\bar{\mu}}$. Furthermore the choice for $\psi^{(-)}_{\bar{\mu}}$ in equation (I–36) is consistent with the case corresponding to a uniform value of ψ within $V(t)$. The form (I–36) is a reflection of the potential discontinuity of ψ across $A(t)$. Similarly the function $p^*_{\bar{\mu}}$ could exhibit a form dependent, in this case, on the sign of $dV^{\bar{\mu}}/dt$, but there is no compelling reason for making a choice analogous to equation (I–36) since it is not associated with a mass flux across the boundary. I only wish to point out that, if $p^{*}_{\bar{\mu}}$ is positive, then $p^{*}_{\bar{\mu}}\, dV^{\bar{\mu}}/dt$ is negative for $dV^{\bar{\mu}}/dt<0$, and this produces an increase in $\langle u \rangle$ as can be seen in equation (I–32). Consequently $-p^{*}_{\bar{\mu}}\, dV^{\bar{\mu}}/dt$ can be thought of as the work done on the contents of V during a reduction of volume. Finally, using equation (I–7) we can show that

$$\dot{H}(t) = \frac{d}{dt}(M\langle p/m \rangle) - p^{*}_{\bar{\mu}} \frac{dV^{\bar{\mu}}}{dt} = \frac{d}{dt}(\rho V \langle p/m \rangle) - p^{*}_{\bar{\mu}} \frac{dV^{\bar{\mu}}}{dt}$$

Because only the weak assumptions (eqs. (I–28) and (I–29)) were used in deriving the ordinary differential equations (I–32) to (I–35), these equations should be applicable to a wide range of problems. The assumption (I-36) merely represents a convenient restriction on the allowed choices for the modeling function $\tilde{\psi}_{\bar{\mu}}$ and may be altered at any time. This choice was made so that the resulting differential equations could be given conventional physical interpretations. The actual use of equations (I–32) to (I–35) and (I–19) only requires the assumption that $\langle u \rangle$, $\langle h \rangle$, $\langle n_\lambda \rangle$, and $\langle \Theta \rangle$ are interrelated by the usual thermodynamic formulas and the specification of the modeling functions which appear in these equations. All geometric aspects of the problem are now confined to the modeling functions. These functions must be chosen so as to reflect properly the geometry in order to carry out a successful modeling calculation.

General steady state equations. – Usually the term "steady state" signifies the absence of temporal derivatives and implies the presence of spatial derivatives alone. Yet sometimes the ordinary one-dimensional, steady state equations are written with time as the independent variable. This is accomplished by a simple change of variable involving a velocity. My objective in this section is to derive generalizations of the ordinary one-dimensional, steady state differential equations for flowing systems. Since I shall not assume that temporal derivatives vanish, time will arise as the independent variable in quite a natural way. Generally, to avoid confusion, one is always careful to use different symbols for different physical quantities. However, to point up the similarity of the steady state equations and the transient equations, I shall violate that convention. In this section some of the symbols used in the preceding section will be applied to different, but similar, quantities. This should cause no confusion since the two sections are independent. Suppose ψ is as defined in the previous section, but suppose that $\langle \psi \rangle$ and M, given in equations (I–14) and (I–15), are redefined here as surface averages (fig. 3) rather than as volume averages.

$$\begin{aligned} \langle \psi \rangle &\equiv \frac{1}{M} \int_{A(\phi,t)} m\psi \, da \\ M(\phi,t) &\equiv \int_{A(\phi,t)} m \, da \end{aligned} \qquad \text{(I–37)}$$

Note that both $\langle \psi \rangle$ and M are now functions of ϕ as well as t, and consequently their derivatives are partial derivatives. It follows from equations (I–37) and the Leibnitz relations (I–9) and (I–10) that

$$\frac{\partial \langle \psi \rangle}{\partial t} = \frac{1}{M}\left[\int_{A(\phi,t)} \frac{\partial (m\psi)}{\partial t} da + \int_{C(\phi,t)} m\psi V^{\alpha}\eta_{\alpha}\, dc\right] - \langle \psi \rangle \frac{1}{M}\frac{\partial M}{\partial t} \qquad \text{(I–38)}$$

$$\frac{\partial \langle \psi \rangle}{\partial \phi} = \frac{1}{M}\int_{C(\phi,t)} m\psi W^{\alpha}\eta_{\alpha}\, dc - \langle \psi \rangle \frac{1}{M}\frac{\partial M}{\partial \phi} \qquad \text{(I–39)}$$

since $\partial(m\psi)/\partial\phi$ is zero because m and ψ have no explicit ϕ dependence. If the conservation equation (I–13) is used in equation (I–38), then we find

$$\frac{\partial \langle \psi \rangle}{\partial t} = \frac{1}{M}\left\{\int_{A(\phi,t)} [S - \nabla_k (m\psi v^k)]\, da + \int_{C(\phi,t)} m\psi V^{\alpha}\eta_{\alpha}\, dc\right\} - \langle \psi \rangle \frac{1}{M}\frac{\partial M}{\partial t} \qquad \text{(I–40)}$$

Just as $\psi = 1$, $S = 0$ produced equation (I-17) as a special case of equation (I-16), this choice in equations (I-39) and (I-40) gives

$$\begin{gathered} \frac{\partial M}{\partial \phi} = \int_{C(\phi,t)} m W^{\alpha} \eta_{\alpha} \, dc \\ \frac{\partial M}{\partial t} = \int_{C(\phi,t)} m V^{\alpha} \eta_{\alpha} \, dc - \int_{A(\phi,t)} \nabla_k (m v^k) \, da \end{gathered} \tag{I-41}$$

Replacement of the partial derivatives (I-38) and (I-39) by ordinary derivatives is possible only when one of the derivatives, say $\partial \langle \psi \rangle / \partial \phi$, vanishes or when ϕ and t can be regarded as dependent. Hence suppose

$$\phi(x^k, t) = \phi = \Phi(t) \tag{I-42}$$

and $d\Phi/dt \equiv \dot{\Phi}$. Then

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \dot{\Phi} \frac{\partial}{\partial \phi} \tag{I-43}$$

and if $\dot{\Phi} \neq 0$, we also have

$$\frac{d}{d\phi} = \frac{1}{\dot{\Phi}} \frac{d}{dt} = \frac{\partial}{\partial \phi} + \frac{1}{\dot{\Phi}} \frac{\partial}{\partial t} \tag{I-44}$$

Since $\dot{\Phi}$ is a function of t alone, we can use equations (I-39) to (I-41) to write dM/dt and $d\langle \psi \rangle / dt$ in the form

$$\frac{dM}{dt} = \int_{C(\Phi,t)} m (V^{\alpha} + \dot{\Phi} W^{\alpha}) \eta_{\alpha} \, dc - \int_{A(\Phi,t)} \nabla_k (m v^k) \, da \tag{I-45}$$

$$\frac{d\langle \psi \rangle}{dt} = \frac{1}{M} \left\{ \int_{A(\Phi,t)} [S - \nabla_k (m \psi v^k)] da + \int_{C(\Phi,t)} m \psi (V^{\alpha} + \dot{\Phi} W^{\alpha}) \eta_{\alpha} \, dc - \langle \psi \rangle \frac{dM}{dt} \right\} \tag{I-46}$$

We now make an assumption analogous to equation (I-29).

$$\frac{dM}{dt} + \int_{A(\Phi,t)} \nabla_k (m v^k) \, da = \int_{C(\Phi,t)} m (V^{\alpha} + \dot{\Phi} W^{\alpha}) \eta_{\alpha} \, dc = 0 \tag{I-47}$$

if and only if

$$\int_{C(\Phi,t)} m \psi (V^{\alpha} + \dot{\Phi} W^{\alpha}) \eta_{\alpha} \, dc = 0$$

Then by analogy with equation (I-31) we now define $\tilde{\psi}$ by

$$\tilde{\psi} \left[\frac{dM}{dt} + \int_{A(\Phi,t)} \nabla_k (m v^k) \, da \right] \equiv \int_{C(\Phi,t)} m \psi (V^{\alpha} + \dot{\Phi} W^{\alpha}) \eta_{\alpha} \, dc \tag{I-48}$$

The substitution of equation (I-48) into equation (I-46) and the recognition that $\tilde{\psi}$ is a function of t alone gives

$$\frac{d\langle\psi\rangle}{dt}=\frac{1}{M}\int_{A(\Phi,t)}\Big\{S-\nabla_k[mv(\psi-\tilde{\psi})]\Big\}da+[\tilde{\psi}-\langle\psi\rangle]\frac{1}{M}\frac{dM}{dt} \tag{I–49}$$

Now we need only make some special choices for ψ to obtain the desired equations. However, before doing that let us try to find a replacement function for M which can be given a simpler physical interpretation. An average density on the surface A can be defined as

$$\rho=\frac{M}{A}=\frac{1}{A(\Phi,t)}\int_{A(\Phi,t)}m\,da \tag{I–50}$$

Now suppose we write $\dot{\mathfrak{M}}$ for the mass flux through the surface A.

$$\dot{\mathfrak{M}}\equiv\int_{A(\Phi,t)}mv^kn_k\,da \tag{I–51}$$

If we write $w\equiv v^kn_k$ for the normal component of the velocity, then w is a permissible choice for ψ and hence

$$\langle w\rangle=\frac{1}{M}\int_{A(\Phi,t)}mv^kn_k\,da \tag{I–52}$$

The combination of the last three equations shows

$$\rho A\langle w\rangle=\dot{\mathfrak{M}} \tag{I–53}$$

and by differentiation

$$\frac{1}{\rho}\frac{d\rho}{dt}+\frac{1}{A}\frac{dA}{dt}+\frac{1}{\langle w\rangle}\frac{d\langle w\rangle}{dt}=\frac{1}{\dot{\mathfrak{M}}}\frac{d\dot{\mathfrak{M}}}{dt} \tag{I–54}$$

Equations (I–53) and (I–54) are the conventional forms of mass conservation used in one-dimensional, steady state flow problems. Furthermore since $\dot{\mathfrak{M}}=M\langle w\rangle$, it is clear that M can always be replaced by the physically more significant mass flux. To determine the differential equation for $\langle w\rangle$, we need the evolution equation for w. This is easily obtained from the evolution equation (I–5) for the velocity v^k and the continuity equation (I–2).

$$\frac{\partial(mw)}{\partial t}+\nabla_k(mwv^k)=n_kF^k+mv^k\frac{\delta n_k}{\delta t} \tag{I–55}$$

Finally we are in a position to obtain the steady state equations with relatively little additional effort. All that is required is to set ψ equal to u, h, n_λ, Θ, and w and to use equations (I–1), (I–6), (I–3), (I–4), and (I–55) to determine the corresponding source term S.

$$\rho\frac{d\langle u\rangle}{dt}=-\dot{Q}(t)+\rho(\tilde{u}-\langle u\rangle)\frac{1}{M}\frac{dM}{dt} \tag{I–56}$$

$$\rho\frac{d\langle h\rangle}{dt}=-\dot{Q}(t)+\dot{H}(t)+\rho(\tilde{h}-\langle h\rangle)\frac{1}{M}\frac{dM}{dt} \tag{I–57}$$

$$\rho\frac{d\langle n_\lambda\rangle}{dt}=\frac{1}{A(\Phi,t)}\int_{A(\Phi,t)}R_\lambda\,da-\dot{N}_\lambda(t)+\rho(\tilde{n}_\lambda-\langle n_\lambda\rangle)\frac{1}{M}\frac{dM}{dt} \tag{I–58}$$

$$\rho \frac{d\langle \Theta \rangle}{dt} = \dot{Q}(t) + \dot{K}(t) + \rho(\tilde{\Theta} - \langle \Theta \rangle) \frac{1}{M} \frac{dM}{dt} \tag{I–59}$$

$$\rho \langle w \rangle \frac{d\langle w \rangle}{dt} + \dot{P}(t) = \rho \langle w \rangle (\tilde{w} - \langle w \rangle) \frac{1}{M} \frac{dM}{dt} \tag{I–60}$$

The functions $Q(t)$, $H(t)$, $N(t)$, $K(t)$, and $P(t)$ are defined by

$$\frac{dQ}{dt} = \dot{Q}(t) \equiv -\frac{1}{A(\Phi,t)} \int_{A(\Phi,t)} \left\{ \Delta \tau^{kj} \nabla_j v_k - m \frac{\partial \Omega}{\partial t} + v^k (\nabla_k p - f_k) - \nabla_k [q^k + \hat{\mu}^\lambda d_\lambda^k + m v^k (h - \tilde{u})] \right\} da \tag{I–61}$$

$$\frac{dH}{dt} = \dot{H}(t) \equiv \frac{1}{A(\Phi,t)} \int_{A(\Phi,t)} \left\{ \frac{\partial p}{\partial t} + \nabla_k [m v^k (\tilde{h} - \tilde{u})] \right\} da \tag{I–62}$$

$$\frac{dN_\lambda}{dt} = \dot{N}_\lambda(t) \equiv \frac{1}{A(\Phi,t)} \int_{A(\Phi,t)} \nabla_k [d_\lambda^k + m v^k (n_\lambda - \tilde{n}_\lambda)] da \tag{I–63}$$

$$\frac{dK}{dt} = \dot{K}(t) \equiv -\frac{1}{A(\Phi,t)} \int_{A(\Phi,t)} \nabla_k [q^k + \hat{\mu}^\lambda d_\lambda^k + m v^k (h - \tilde{u} + \Theta - \tilde{\Theta}) - v_i \Delta \tau^{ik}] da \tag{I–64}$$

$$\frac{dP}{dt} = \dot{P}(t) \equiv -\frac{\langle w \rangle}{A(\Phi,t)} \int_{A(\Phi,t)} \left\{ n_k F^k + m v^k \frac{\delta n_k}{\delta t} - \nabla_k [m v^k (w - \tilde{w})] \right\} da \tag{I–65}$$

In the steady state equations, as in the transient equations, all geometric considerations are concealed in the modeling functions. The definitions of these functions (eqs. (I–45) and (I–61) to (I–65) can be rewritten somewhat by separating out the contribution of fluxes through the tube surface. If the intrinsic coordinates of the subspace containing $A(\Phi,t)$ are y^α and the coordinates of the three space are x^k, then the subspace can be characterized by functions $x^k = x^k(y^\alpha)$. The covariant components of the metric tensor $b_{\alpha\beta}$ of the subspace are expressed in terms of the covariant components of the metric tensor g_{kj}

$$b_{\alpha\beta} = \left(\frac{\partial x^k}{\partial y^\alpha} \right) \left(\frac{\partial x^j}{\partial y^\beta} \right) g_{kj}$$

If $b^{\alpha\beta}$ are the contravariant components of the subspace metric, then we can define $B_k^\alpha \equiv b^{\alpha\gamma} (\partial x^j / \partial y^\gamma) g_{jk}$ and write $B_\alpha^k \equiv \partial x^k / \partial y^\alpha$. These two quantities satisfy $B_\alpha^k B_k^\gamma = \delta_\alpha^\gamma$, where δ_α^γ is a Kronecker delta, and they can be used to define the projection operator P_j^k, for the subspace by $P_j^k \equiv B_\alpha^k B_j^\alpha$. Now for any vector, say g^k, it can be shown that

$$\nabla_\alpha g^\gamma - B_i^\gamma B_\alpha^j \nabla_j g^i = (g^k - P_j^k g^j) \left(\frac{\partial B_k^\gamma}{\partial y^\alpha} - B_i^\gamma B_\alpha^l \left\{ {i \atop lk} \right\} \right)$$

where $g^\gamma = B_i^\gamma g^i$ and $\left\{ {i \atop lk} \right\}$ are the Christoffel symbols of the second kind for the three space. From this it follows that we can write

$$\nabla_i g^i = \nabla_\alpha g^\alpha + (\nabla_i g^i - \nabla_\alpha g^\alpha) = \nabla_\alpha g^\alpha + (\delta_i^j - P_i^j) \left[\nabla_j g^i - g^i \left(\frac{\partial B_j^\alpha}{\partial y^\alpha} - P_k^l \left\{ {k \atop lj} \right\} \right) \right]$$

If we now apply Green's theorem in the subspace, then

$$\frac{1}{A(\Phi,t)}\int_{A(\Phi,t)} \nabla_i g^i \, da = \frac{C(\Phi,t)}{A(\Phi,t)}\,\frac{1}{C(\Phi,t)}\int_{C(\Phi,t)} g^\alpha \eta_\alpha \, dc$$
$$+\frac{1}{A(\Phi,t)}\int_{A(\Phi,t)} (\delta^j_i - P^j_i)\left[\nabla_j g^i - g^i\left(\frac{\partial B^\alpha_j}{\partial y^\alpha} - P^l_k\left\{ {k \atop lj} \right\}\right)\right] da$$

This formula can now be applied to all divergence terms in the definitions (I–45) and (I–61) to (I–65) to separate the fluxes through the tube surfaces from the other contributions. While this rewriting is not significant for the further developments in this report, it should facilitate the writing of suitable functions to model the quantities defined in equations (I–45) and (I–61) to (I–65). In this same vein, as I have previously indicated, it might be desirable to replace M by the more meaningful $\mathfrak{M}$. In particular, it is the combination $M^{-1}\, dM/dt$ which appears in equations (I–56) to (I–60). An expression for this factor can readily be obtained by differentiating $\mathfrak{M} = M\langle w\rangle$ and eliminating $d\langle w\rangle/dt$ between this equation and (I–60).

$$\frac{1}{M}\frac{dM}{dt} = \frac{\langle w\rangle}{\tilde{w}}\left(\frac{1}{\mathfrak{M}}\frac{d\mathfrak{M}}{dt} + \frac{\dot{P}}{\rho\langle w\rangle^2}\right)$$

This may be used in equations (I–56) to (I–60), and it eliminates the need to specify dM/dt. When this substitution is made into equation (I–60), we find

$$\rho\langle w\rangle\frac{d\langle w\rangle}{dt} + \dot{P}(t) = \rho\langle w\rangle^2\left(\frac{\tilde{w}-\langle w\rangle}{\tilde{w}}\right)\left(\frac{1}{\mathfrak{M}}\frac{d\mathfrak{M}}{dt} + \frac{\dot{P}}{\rho\langle w\rangle^2}\right)$$

It is apparent that a considerable simplification in this differential equation is achieved if the right side vanishes for then it reduces to the usual form of the one-dimensional "momentum" equation. Since on physical grounds $\rho\langle w\rangle^2$ is positive, we see that

$$\rho\langle w\rangle\frac{d\langle w\rangle}{dt} + \dot{P}(t) = 0$$

if and only if $\tilde{w} = \langle w\rangle$ or

$$\frac{1}{\mathfrak{M}}\frac{d\mathfrak{M}}{dt} + \frac{\dot{P}}{\rho\langle w\rangle^2} = 0$$

Similarly the addition of equation (I–57) to equation (I–59) gives a differential equation from which we easily deduce the analog of energy conservation in flow systems.

$$\frac{d}{dt}[\langle h\rangle + \langle\Theta\rangle] = \dot{e}(t)$$
$$\rho\dot{e}(t) \equiv \dot{H}(t) + \dot{K}(t) + \rho[(\tilde{h}+\tilde{\Theta}) - (\langle h\rangle + \langle\Theta\rangle)]\frac{1}{M}\frac{dM}{dt} \qquad \text{(I–66)}$$

where $\langle h\rangle + \langle\Theta\rangle =$ constant if and only if $\dot{e}(t) = 0$.

Unlike the usual steady state equations, the equations of this section involve two scalar velocities, namely, the normal component $v^k n_k = w$ and $v^k v_k = v^2$. Since w^2 is not necessarily equal to v^2, there is no reason to expect that $\langle v^2\rangle$ will equal $\langle w\rangle^2$ or to insist that $\widetilde{v^2}$ equal $\tilde{w}^2$. Indeed, the subtraction of equation (I–60) from equation (I–59) gives

$$\frac{\rho}{2}\frac{d}{dt}(\langle v^2\rangle-\langle w\rangle^2)=\dot{P}+\dot{Q}+\dot{K}+\rho[\tilde{\Theta}-\langle\Theta\rangle-\langle w\rangle(\tilde{w}-\langle w\rangle)]\frac{1}{M}\frac{dM}{dt}-\rho\frac{d\langle\Omega\rangle}{dt}$$

$$=\dot{P}+\dot{Q}+\dot{K}+\rho\left\{\frac{\widetilde{v^2}-\tilde{w}^2}{2}-\frac{\langle v^2\rangle-\langle w\rangle^2}{2}+\frac{[\langle w\rangle-\tilde{w}]^2}{2}+\tilde{\Omega}-\langle\Omega\rangle\right\}\frac{1}{M}\frac{dM}{dt}$$

$$-\rho\frac{d\langle\Omega\rangle}{dt}$$

Thus from this differential equation follows the theorem that $\langle v^2\rangle=\langle w\rangle^2$ if and only if $\langle v^2\rangle$ equals $\langle w\rangle^2$ for some t and

$$\dot{P}+\dot{Q}+\dot{K}+\frac{\rho}{2}\left\{(\widetilde{v^2}-\tilde{w}^2)+(\langle w\rangle-\tilde{w})^2+2(\tilde{\Omega}-\langle\Omega\rangle)\right\}\frac{1}{M}\frac{dM}{dt}-\rho\frac{d\langle\Omega\rangle}{dt}=0$$

This represents a constraint on the modeling functions which one may or may not wish to impose, but it certainly can be satisfied in many ways. Obviously it could be written in terms of $\dot{\mathfrak{M}}^{-1}\, d\dot{\mathfrak{M}}/dt$ by substituting for $M^{-1}\, dM/dt$. The imposition of the conditions

$$\frac{d\dot{\mathfrak{M}}}{dt}=0,\ P=\langle p\rangle,\ \tilde{w}=\langle w\rangle,\ \dot{N}_\lambda=\frac{(\tilde{n}_\lambda-\langle n_\lambda\rangle)\dot{P}}{\langle w\rangle^2}$$

$$\dot{P}+\dot{Q}+\dot{K}+\frac{1}{2}\left\{\widetilde{v^2}-\tilde{w}^2+2(\tilde{\Omega}-\langle\Omega\rangle)\right\}\frac{\dot{P}}{\langle w\rangle^2}-\rho\frac{d\langle\Omega\rangle}{dt}=0,\ \dot{P}+\dot{Q}=\dot{H}+\frac{(\tilde{h}-\langle h\rangle)\dot{P}}{\langle w\rangle^2}$$

on the general steady state equations of this section, together with the assumption that ρ, $\langle u\rangle$, $\langle h\rangle$, $\langle p\rangle$, and $\langle n_\lambda\rangle$ are interrelated by the usual thermodynamic formulas and that $A^{-1}\int_A R_\lambda\, da$ is modeled by the usual rate expressions, produces the conventional steady state equations. These are

$$\frac{d\dot{\mathfrak{M}}}{dt}=0,\ \rho A\langle w\rangle=\dot{\mathfrak{M}},\ \rho\langle w\rangle\frac{d\langle w\rangle}{dt}+\frac{d\langle p\rangle}{dt}=0$$

$$\rho\frac{d\langle n_\lambda\rangle}{dt}=A^{-1}\int_A R_\lambda\, da,\ \langle h\rangle+\frac{\langle w\rangle^2}{2}=\text{constant}$$

The function $\dot{e}(t)$ defined in equation (I–66) usually will be nonzero, and a simple quadrature of the differential equation in (I–66) establishes that

$$\langle h\rangle_2+\langle\Theta\rangle_2-(\langle h\rangle_1+\langle\Theta\rangle_1)=\Delta e=e(t_2)-e(t_1)=\int_{t_1}^{t_2}\dot{e}(t)\,dt$$

But if $\Gamma\equiv\langle v^2\rangle/\langle w\rangle^2$, then this equation can be reexpressed as

$$\Gamma_2(\langle w\rangle_2)^2-\Gamma_1(\langle w\rangle_1)^2=2\left\{\Delta e-[\langle h\rangle_2+\langle\Omega\rangle_2-(\langle h\rangle_1+\langle\Omega\rangle_1)]\right\}$$

If this equation is supplemented by an equation for the increment in $\dot{\mathfrak{M}}$

$$\rho_2A_2\langle w\rangle_2-\rho_1A_1\langle w\rangle_1=\Delta\dot{\mathfrak{M}}\equiv\dot{\mathfrak{M}}_2-\dot{\mathfrak{M}}_1$$

then this pair of equations can be solved simultaneously for $\langle w \rangle_2$, in terms of Γ_1, Γ_2, Δe, and $\Delta\dot{\mathfrak{M}}$. This can then be used to calculate $\dot{\mathfrak{M}}_2$ and from it $\dot{\mathfrak{M}}_1$.

$$\dot{\mathfrak{M}}_1 = \left(\frac{\Gamma_1\rho_2^2A_2^2}{\Gamma_2\rho_1^2A_1^2} - 1\right)^{-1} \Delta\dot{\mathfrak{M}} + \rho_1A_1\left\{\left(\frac{\rho_2A_2}{\rho_1A_1}\right)^2\left[2\Gamma_2^{-1}\left(1 - \frac{\Gamma_1\rho_2^2A_2^2}{\Gamma_2\rho_1^2A_1^2}\right)^{-1}\right.\right.$$
$$\times(\Delta e - \langle h \rangle_2 - \langle \Omega \rangle_2 + \langle h \rangle_1 + \langle \Omega \rangle_1)$$
$$\left.\left. + \left(\frac{\Gamma_1\rho_2^2A_2^2}{\Gamma_2\rho_1^2A_1^2}\right)\left(1 - \frac{\Gamma_1\rho_2^2A_2^2}{\Gamma_2\rho_1^2A_1^2}\right)^{-2}\left(\frac{\Delta\dot{\mathfrak{M}}}{\rho_2A_2}\right)^2\right]\right\}^{1/2} \tag{I-67}$$

If $\Delta\dot{\mathfrak{M}}$ equals 0, Δe equals 0, and $\langle h \rangle_2 - \langle h \rangle_1$ is replaced by its approximation for an isentropic process in an ideal gas, then this equation reduces to the steady state flow equation, which is used as the basis for flowmetering. A generalization with the same basic form, valid even if $\Delta e \neq 0$ and the flow is nonisentropic, can be obtained from equation (I-67) with $\Delta\dot{\mathfrak{M}} = 0$ and no other approximations. Suppose we consider a thermodynamic process characterized by the curve

$$p = k\rho^{\kappa} \tag{I-68}$$

where k and κ are constants. For such a curve it is true that

$$-\Delta q = -(q_2 - q_1) \equiv \int_{p_2}^{p_1} \rho^{-1}\,dp = \begin{cases} \kappa(\kappa-1)^{-1}p_1\rho_1^{-1}\left[1 - \left(\dfrac{p_2}{p_1}\right)^{(\kappa-1)/\kappa}\right] & \kappa \neq 1 \\ p_1\rho_1^{-1}\ln\left(\dfrac{p_1}{p_2}\right) & \kappa = 1 \end{cases} \tag{I-69}$$

If the constant κ is taken to be the isentropic exponent $\gamma \equiv (\partial \ln p/\partial \ln \rho)_s$ for an ideal gas, then the curve is an isentrope and for such a case $\Delta q = \langle h \rangle_2 - \langle h \rangle_1$. Using only the form of Δq given in equation (I-69) together with equation (I-68) and the assumption $\Delta\dot{\mathfrak{M}} = 0$, we can write $\dot{\mathfrak{M}}_1$ exactly in the form

$$\dot{\mathfrak{M}}_1 = \begin{cases} \rho_1A_2\Gamma_2^{-1/2}\left(\dfrac{\rho_2}{\rho_1}\right)\left(\dfrac{p_1}{p_2}\right)^{1/\kappa}\left\{\dfrac{2p_1\rho_1^{-1}\kappa(\kappa-1)^{-1}[\sigma - (p_2/p_1)^{(\kappa-1)/\kappa}]}{(p_1/p_2)^{2/\kappa} - (\Gamma_1A_2^2/\Gamma_2A_1^2)(\rho_2p_1^{1/\kappa}/\rho_1p_2^{1/\kappa})^2}\right\}^{1/2} & \kappa \neq 1 \\ \rho_1A_2\Gamma_2^{-1/2}\left(\dfrac{\rho_2}{\rho_1}\right)\left(\dfrac{p_1}{p_2}\right)^{1/\kappa}\left\{\dfrac{2p_1\rho_1^{-1}(\sigma + \ln p_1/p_2)}{(p_1/p_2)^{2/\kappa} - (\Gamma_1A_2^2/\Gamma_2A_1^2)(\rho_2p_1^{1/\kappa}/\rho_1p_2^{1/\kappa})^2}\right\}^{1/2} & \kappa = 1 \end{cases} \tag{I-70}$$

where σ is defined as

$$\sigma = \begin{cases} 1 + \dfrac{(\Delta e + \langle \Omega \rangle_1 - \langle \Omega \rangle_2 + \langle h \rangle_1 - \langle h \rangle_2 + \Delta q)(\kappa - 1)}{\kappa p_1\rho_1^{-1}} & \kappa \neq 1 \\ \dfrac{(\Delta e + \langle \Omega \rangle_1 - \langle \Omega \rangle_2 + \langle h \rangle_1 - \langle h \rangle_2 + \Delta q)}{p_1\rho_1^{-1}} & \kappa = 1 \end{cases} \tag{I-71}$$

Even though the equations of this section have been called the steady state equations, they are not restricted to steady state phenomena. Steady state phenomena are characterized by the vanishing of all temporal derivatives, and that assumption has certainly not been made. Both the function $\phi(x^k, t)$ and the function $\Phi(t)$ may depend explicitly on time. Suppose that the function $\phi(x^k, t)$ is chosen to be a solution of the equation

$$\frac{\partial \phi}{\partial t}+A^k \nabla_k \phi=0$$

where A^k is some velocity. If $A^k=v^k$, then the surfaces of constant ϕ propagate with the flow, and hence the fluid particles on a given surface always remain on the same surface although the surface itself propagates and deforms as a result of the flow. To use the velocity v^k in such a manner implies that the flow field has already been determined or else prescribed.

Should it be desirable to employ a distance as the independent variable rather than time, then this can readily be done. Suppose we define a distance variable r by

$$r=r_o+\int_{t_o}^{t} \langle w \rangle \, dt'$$

where r_o and t_o are constants. Then $d/dt=(dr/dt)\ d/dr=\langle w \rangle\ d/dr$ and hence

$$\frac{d}{dr}=\frac{1}{\langle w \rangle}\frac{d}{dt}$$

If we were also to make the choice $\dot{\Phi}(t)=\langle w \rangle$, then $\Phi(t)$ equals $r+\Phi(t_o)-r_o$, and hence from equation (I-42) we obtain $\phi=r+\Phi(t_o)-r_o$ and thus

$$\frac{d}{d\phi}=\frac{d}{dr}$$

Any other velocity which depends on t alone could be used similarly to introduce a distance variable.

Conclusions. – Let us recapitulate the results of the preceding two sections. Under relatively weak assumptions I have derived ordinary differential equations which can be used in the modeling of reacting fluid systems. One system of equations (eqs. (I-19) and (I-32) to (I-35)) corresponds to a generalization of the usual transient equations for spatially homogeneous systems, while the other system of equations (eqs. (I-54) and (I-56) to (I-60)) is a generalization of the usual steady state, one-dimensional flow equations. These equations were obtained without the assumption of any kind of spatial uniformity, without the requirement that temporal derivatives vanish, and without neglecting dissipative and transport effects. The derivation did use the partial differential equations governing the evolution of fluid systems, but no assumptions were made about the form of the constitutive relations. In both cases the boundaries of the physical system may be movable and permeable to heat and mass. There is a significant corollary to the two systems of equations and the fact that chemical kinetics experiments are usually analyzed for rate constants by ordinary differential equations. In the transient case the modeling function for the species production rate represents the volumetric average of the local production rate, while in the steady state case it is the surface average. These two averages cannot be expected to coincide with each other or with the local production rate except when we have uniform conditions within the volume or on the surface. Since experimental systems used to measure rate constants may exhibit compositional nonuniformities, the two types of experiments can be expected to give different rate constants. Finally, let me point out that in the application of the differential equations to physical problems it may be desirable to use various combinations of the two systems of equations.

Specialization of Differential Equations for the Internal Combustion Engine

The Otto cycle can be decomposed into two distinctly different phases of operation: the combustion phase, characterized by the presence of a propagating flame front, and the noncombustion phase, identified by the absence of a flame front. The combustion phase begins with the ignition of the combustible working fluid by the spark plug and terminates when the flame has completely engulfed the combustible working fluid. Of course, the completion of the combustion phase does not signal an end to chemical reaction for this continues during the following noncombustion phase. Flow in the intake or exhaust systems can alter the amount of working fluid during either phase of the cycle.

A set of equations for each phase can be written from the equations just derived; however, it will be convenient to alter some of the notation used there. Only tensors of rank zero, namely scalars, will be encountered from now on. Thus Latin indices will no longer be tensor indices but may be used for any other labeling purpose. Angular brackets, $\langle\rangle$, which were used to distinguish between a local property and its average over a region of space are no longer necessary; henceforth we shall always be dealing with average properties and consequently the use of angular brackets will be discontinued. It will also be convenient to assign a new meaning to the labels $(\pm)$ which appeared in equation (I–36). From now on the label $(+)$ will refer to the intake system while $(-)$ will designate the exhaust system and this notation will be used in place of the barred Greek indices. At the piston face the barred Greek index will be suppressed entirely. Finally, the volume average of the volumetric species production rate will be simply written as R_λ. The customary choice for the independent variable is the crankangle, $\theta=\theta(t)$, where $\theta=0$ corresponds to minimum cylinder volume, top dead center. The crankangle is then incremented by 4π radians per cycle although its value is commonly given modulo 4π. The transformation from time to crankangle introduces the angular frequency $\omega=d\theta/dt$ into the equations. These notational alterations, when applied to the transient equations (I–19) and (I–32) to (I–35), yield the differential equations for the noncombustion phase.

$$\begin{aligned}
&\frac{d\ln\rho}{d\theta}=\frac{d\ln M}{d\theta}-\frac{d\ln V}{d\theta}\\
&\frac{du}{d\theta}=M^{-1}\left[-p^*\frac{dV}{d\theta}+\tilde{h}^{(+)}\frac{dM^{(+)}}{d\theta}+\tilde{h}^{(-)}\frac{dM^{(-)}}{d\theta}-u\frac{dM}{d\theta}-\frac{\dot{Q}}{\omega}\right]\\
&\frac{dn_\lambda}{d\theta}=\frac{R_\lambda}{\rho\omega}+M^{-1}\left[\tilde{n}_\lambda^{(+)}\frac{dM^{(+)}}{d\theta}+\tilde{n}_\lambda^{(-)}\frac{dM^{(-)}}{d\theta}-n_\lambda\frac{dM}{d\theta}-\frac{\dot{N}_\lambda}{\omega}\right]\\
&\frac{d\Theta}{dt}=M^{-1}\left[\tilde{\Theta}^{(+)}\frac{dM^{(+)}}{d\theta}+\tilde{\Theta}^{(-)}\frac{dM^{(-)}}{d\theta}-\Theta\frac{dM}{d\theta}+\frac{\dot{Q}}{\omega}+\frac{\dot{K}}{\omega}\right]\\
&\frac{dM}{d\theta}=\frac{dM^{(+)}}{d\theta}+\frac{dM^{(-)}}{d\theta},\quad \frac{dM^{(+)}}{d\theta}=\dot{M}^{(+)},\quad \frac{dM^{(-)}}{d\theta}=\dot{M}^{(-)}
\end{aligned}\tag{I–72}$$

The first four of these equations correspond to (I–19), (I–32), (I–34) and (I–35). Built into these equations is the assumption that mass can enter or leave the cylinder only through the intake and exhaust systems; blow-by of gases past the piston is neglected. Also I have assumed that the cylinder volume is altered only by piston motion, that is, $dV^{(+)}/d\theta=0$ and $dV^{(-)}/d\theta=0$. These equations (I–72) are supplemented by the assumption that u, ρ, and n_λ are related to all other thermodynamic quantities by the usual thermodynamic expressions. This enables us to obtain differential equations for the other thermodynamic quantities from those for u, ρ, and n_λ. For example, we know that $u=u(T,\rho,n_\lambda)$ and we obtain, by differentiation, a relationship among derivatives.

$$\frac{du}{d\theta}=\frac{\partial u}{\partial T}\frac{dT}{d\theta}+\frac{\partial u}{\partial\rho}\frac{d\rho}{d\theta}+\frac{\partial u}{\partial n_\lambda}\frac{dn_\lambda}{d\theta}\tag{I–73}$$

This immediately becomes an equation for T if $du/d\theta$, $d\rho/d\theta$, and $dn_\lambda/d\theta$ are eliminated with equation (I–72) and the resulting equation could be used in place of the equation for u.

The equations become considerably more complex for the combustion phase and so too does their description. During combustion the working fluid is assumed to be partitioned into burned and unburned gases by a flame zone whose material and energy content may be neglected. The sole function of the flame zone is to establish the partition and initiate chemical reactions in the working fluid as it passes through the flame zone. The burned working fluid is labeled with a 1 and the unburned with a 2. The intake and exhaust system continue to be designated by (+) and (−) and the flame zone region with b.

$$\begin{aligned}
&\frac{d\ln\rho_1}{d\theta}=\frac{d\ln M_1}{d\theta}-\frac{d\ln V_1}{d\theta}\\
&\frac{du_1}{d\theta}=M_1^{-1}\left[-p_1^*\frac{dV_1}{d\theta}+\tilde{h}_1^{(+)}\frac{dM_1^{(+)}}{d\theta}+\tilde{h}_1^{(-)}\frac{dM_1^{(-)}}{d\theta}+\tilde{h}_1^{(b)}\frac{dM_1^{(b)}}{d\theta}-u_1\frac{dM_1}{d\theta}-\frac{\dot{Q}_1}{\omega}\right]\\
&\frac{dn_\lambda^{(1)}}{d\theta}=\frac{R_\lambda^{(1)}}{\rho_1\omega}+M_1^{-1}\left[\tilde{n}_\lambda^{(1,+)}\frac{dM_1^{(+)}}{d\theta}+\tilde{n}_\lambda^{(1,-)}\frac{dM_1^{(-)}}{d\theta}+\tilde{n}_\lambda^{(1,b)}\frac{dM_1^{(b)}}{d\theta}-n_\lambda^{(1)}\frac{dM_1}{d\theta}-\frac{\dot{N}^{(1)}}{\omega}\right]\\
&\frac{d\Theta_1}{d\theta}=M_1^{-1}\left[\tilde{\Theta}_1^{(+)}\frac{dM_1^{(+)}}{d\theta}+\tilde{\Theta}_1^{(-)}\frac{dM_1^{(-)}}{d\theta}+\tilde{\Theta}_1^{(b)}\frac{dM_1^{(b)}}{d\theta}-\Theta_1\frac{dM_1}{d\theta}+\frac{\dot{Q}_1}{\omega}+\frac{\dot{K}_1}{\omega}\right]\\
&\frac{dM_1}{d\theta}=\frac{dM_1^{(+)}}{d\theta}+\frac{dM_1^{(-)}}{d\theta}+\frac{dM_1^{(b)}}{d\theta},\quad \frac{dM_1^{(+)}}{d\theta}=\dot{M}_1^{(+)},\quad \frac{dM_1^{(-)}}{d\theta}=\dot{M}_1^{(-)}\\
&\frac{d\ln\rho_2}{d\theta}=\frac{d\ln M_2}{d\theta}-\frac{d\ln V_2}{d\theta}\\
&\frac{du_2}{d\theta}=M_2^{-1}\left[-p_2^*\frac{dV_2}{d\theta}+\tilde{h}_2^{(+)}\frac{dM_2^{(+)}}{d\theta}+\tilde{h}_2^{(-)}\frac{dM_2^{(-)}}{d\theta}+\tilde{h}_2^{(b)}\frac{dM_2^{(b)}}{d\theta}-u_2\frac{dM_2}{d\theta}-\frac{\dot{Q}_2}{\omega}\right]\\
&\frac{dn_\lambda^{(2)}}{d\theta}=\frac{R_\lambda^{(2)}}{\rho_2\omega}+M_2^{-1}\left[\tilde{n}_\lambda^{(2,+)}\frac{dM_2^{(+)}}{d\theta}+\tilde{n}_\lambda^{(2,-)}\frac{dM_2^{(-)}}{d\theta}+\tilde{n}_\lambda^{(2,b)}\frac{dM_2^{(b)}}{d\theta}-n_\lambda^{(2)}\frac{dM_2}{d\theta}-\frac{\dot{N}^{(2)}}{\omega}\right]\\
&\frac{d\Theta_2}{d\theta}=M_2^{-1}\left[\tilde{\Theta}_2^{(+)}\frac{dM_2^{(+)}}{d\theta}+\tilde{\Theta}_2^{(-)}\frac{dM_2^{(-)}}{d\theta}+\tilde{\Theta}_2^{(b)}\frac{dM_2^{(b)}}{d\theta}-\Theta_2\frac{dM_2}{d\theta}+\frac{\dot{Q}_2}{\omega}+\frac{\dot{K}_2}{\omega}\right]\\
&\frac{dM_2}{d\theta}=\frac{dM_2^{(+)}}{d\theta}+\frac{dM_2^{(-)}}{d\theta}+\frac{dM_2^{(b)}}{d\theta},\quad \frac{dM_2^{(+)}}{d\theta}=\dot{M}_2^{(+)},\quad \frac{dM_2^{(-)}}{d\theta}=\dot{M}_2^{(-)}\\
&\frac{dM_1^{(b)}}{d\theta}=-\frac{dM_2^{(b)}}{d\theta}=\dot{M}_b\geq 0
\end{aligned}\tag{I-74}$$

The first four and the eighth through eleventh members of equation (I-74) were obtained by the application of equations (I-19), (I-32), (I-34), and (I-35) to the burned and unburned parts of the working fluid. I neglected piston blowby and, by again assuming that intake and exhaust valves do not alter volumes, I set $dV_1^{(+)}/d\theta=0=dV_1^{(-)}/d\theta$ and $dV_2^{(+)}/d\theta=0=dV_2^{(-)}/d\theta$. The last member of equation (I-74) imposes the conditions that burned gas is created only at the expense of unburned gas and that the burning rate is never negative. Just as for the noncombustion phase, I assumed that all thermodynamic properties for the burned and unburned working fluids are completely characterized by u_1, ρ_1, $n_\lambda^{(1)}$ and u_2, ρ_2, $n_\lambda^{(2)}$, respectively. Naturally the average values of the corresponding variables for the total working fluid are related to those of the burned and unburned gases in a simple way

$$Mu = M_1 u_1 + M_2 u_2, \quad Mn_\lambda = M_1 n_\lambda^{(1)} + M_2 n_\lambda^{(2)}$$
$$\rho = \frac{M}{V}, \quad M = M_1 + M_2, \quad V = V_1 + V_2 \tag{I-75}$$

The duration of the combustion phase is determined by specifying the values of M_1/M at the start of combustion, $\theta = \theta_0$, and at its conclusion, $\theta = \theta^*$. I shall assume that the initiation of the combustion by a spark produces an initial value of $M_1/M = 10^{-4}$ and that the combustion phase is terminated at a crankangle such that M_1/M would equal 0.9999 if $dM/d\theta$ were zero during combustion.

Hierarchy of Models

General model. – Equations (I-72) to (I-74) become useful tools for predicting the behavior of the internal combustion engine only after the functions on the right sides of equations (I-72) and (I-74) are specified completely. These modeling functions offer us an opportunity to mold these general equations into a descriptive tool for the internal combustion engine with some appropriate specific choices. Those choices are dictated by our experimental and intuitive knowledge about the behavior of real engines. Unfortunately our knowledge of the physical processes taking place in the internal combustion engine is so meager, as I already pointed out in the Introduction, that it is impossible to make definitive choices for the modeling functions. The best one can hope for is the selection of functions, with adjustable parameters, which are capable of accommodating a broad spectrum of behavior. One hopes this broad spectrum will contain the actual behavior as a special case. In this event the parameters contained in the modeling functions could perhaps be determined by a comparison of model calculations with experimental data. However, since the differential equations are nonlinear, it would not be surprising if the parameter set obtained in this manner were not unique.

My choices for the modeling functions will be described in several stages. In this section I shall present those choices which are applicable to the most complex and sophisticated model in the hierarchy of models. Subsequent sections will be devoted to progressively greater specializations of the general model which will yield less detailed, and hence somewhat less realistic, descriptions of the operation of an internal combustion engine. An obvious advantage of a simpler model is that it requires less information to characterize it completely than is necessary for a more detailed model. This permits calculations even in those situations where our knowledge is inadequate to characterize a more sophisticated model.

General assumptions: For the noncombustion phase I have elected to write

$$p^* = p, \quad \dot{Q} = \bar{h} A (T - T_w), \quad \dot{N}_\lambda = 0, \quad \dot{K} = -\dot{Q} + \omega \left[\Theta \frac{dM}{d\theta} - \tilde{\Theta}^{(+)} \frac{dM^{(+)}}{d\theta} - \tilde{\Theta}^{(-)} \frac{dM^{(-)}}{d\theta} \right] \tag{I-76}$$

with similar forms for the combustion phase.

$$\begin{gathered}
p_1^* = p_1, \quad \dot{Q}_1 = \bar{h}_1 \mathrm{A}_1 (T_1 - T_w), \quad \dot{N}_\lambda^{(1)} = 0, \\
\dot{K}_1 = -\dot{Q}_1 + \omega \left[\Theta_1 \frac{dM_1}{d\theta} - \tilde{\Theta}_1^{(+)} \frac{dM_1^{(+)}}{d\theta} - \tilde{\Theta}_1^{(-)} \frac{dM_1^{(-)}}{d\theta} \right], \quad \dot{M}_1^{(+)} = 0 \\
p_2^* = p_2, \quad \dot{Q}_2 = \bar{h}_2 A_2 (T_2 - T_w), \quad \dot{N}_\lambda^{(2)} = 0 = R_\lambda^{(2)} \\
\dot{K}_2 = -\dot{Q}_2 + \omega \left[\Theta_2 \frac{dM_2}{d\theta} - \tilde{\Theta}_2^{(+)} \frac{dM_2^{(+)}}{d\theta} - \tilde{\Theta}_2^{(-)} \frac{dM_2^{(-)}}{d\theta} \right] \\
\dot{M}_2^{(\pm)} = 0, \quad p_1 = p_2, \quad \frac{A_1}{M_1} = \frac{A_2}{M_2} = \frac{A}{M}
\end{gathered} \tag{I-77}$$

The content of equations (I-76) and (I-77) is readily verbalized. The "volume flux average" of the pressure is assumed to be independent of the sign of the appropriate volume rate of change and is made equal to the thermodynamic pressure. The heat flux is taken to be expressible as the product of a heat transfer coefficient, an area, and the temperature difference between the working fluid and some effective wall temperature. The diffusive fluxes of mass are assumed to be unimportant in the determination of composition, and no reactions take place in the unburned gas. The inlet system always remains closed during the combustion phase, and if the exhaust system is open during combustion, flow only affects the burned gas. Hence, $\dot{M}_2^{(\pm)}=0$ and $\dot{M}_1^{(+)}=0$ always hold. Finally the choices for $\dot{K}$, $\dot{K}_1$, and $\dot{K}_2$ imply that Θ, Θ_1, and Θ_2 are constant, and thus their evolution equations can be removed from further consideration. For the combustion phase these conditions are supplemented by the requirement that the pressures of the burned and unburned gases always remain equal and by the assumption that the areas A_1 and A_2 are equal to a mass fraction weighting of the total area. The latter reflects my belief that the flame propagation is geometrically so complex that one can never adequately and unambiguously evaluate the wall areas in contact with the burned and unburned gases. All that one can reasonably expect to know is the total surface area of the cylinder in contact with the working fluid.

The pressure constraint, written as the next to last member of equation (I-77), and the volume constraint, which is the last member of equation (I-75), can be viewed as integrals of the system of equations defining the combustion phase of the cycle. They can be used to define the evolution of the burned and unburned volumes. The pressure can be regarded as a function of internal energy, density, and composition, that is, $p=p(u, \rho, n_\lambda)$. Consequently, by differentiation of the pressure constraint, we obtain a relationship among the derivatives of the internal energy, density, and composition of the burned and unburned gases. Instead of working with the constraint $p_1=p_2$, it is more convenient to deal with its logically equivalent form $\ln p_1=\ln p_2$.

$$\frac{\partial \ln p_1}{\partial u_1}\frac{du_1}{d\theta}+\frac{\partial \ln p_1}{\partial \ln \rho_1}\frac{d\ln \rho_1}{d\theta}+\frac{\partial \ln p_1}{\partial n_\lambda^{(1)}}\frac{dn_\lambda^{(1)}}{d\theta}=\frac{\partial \ln p_2}{\partial u_2}\frac{du_2}{d\theta}+\frac{\partial \ln p_2}{\partial \ln \rho_2}\frac{d\ln \rho_2}{d\theta}+\frac{\partial \ln p_2}{\partial n_\lambda^{(2)}}\frac{dn_\lambda^{(2)}}{d\theta}$$

If the derivatives of u_1, u_2, ρ_1, and ρ_2 with respect to θ are eliminated with the differential equations (I-74), then we obtain a relatively simple relation connecting $dV_1/d\theta$ and $dV_2/d\theta$.

$$\begin{aligned}
&-\left(p_1\rho_1^{-1}\frac{\partial \ln p_1}{\partial u_1}+\frac{\partial \ln p_1}{\partial \ln \rho_1}\right)\frac{d\ln V_1}{d\theta}+\left(p_2\rho_2^{-1}\frac{\partial \ln p_2}{\partial u_2}+\frac{\partial \ln p_2}{\partial \ln \rho_2}\right)\frac{d\ln V_2}{d\theta}\\
&\quad=M_2^{-1}\frac{\partial \ln p_2}{\partial u_2}\left[(\tilde{h}_2^{(+)}-u_2)\dot{M}_2^{(+)}+(\tilde{h}_2^{(-)}-u_2)\dot{M}_2^{(-)}-(\tilde{h}_2^{(b)}-u_2)\dot{M}_b-\frac{\dot{Q}_2}{\omega}\right]\\
&\qquad-\mathrm{M}_1^{-1}\frac{\partial \ln p_1}{\partial u_1}\left[(\tilde{h}_1^{(+)}-u_1)\dot{M}_1^{(+)}+(\tilde{h}_1^{(-)}-u_1)\dot{M}_1^{(-)}+(\tilde{h}_1^{(b)}-u_1)\dot{M}_b-\frac{\dot{Q}_1}{\omega}\right]\\
&\qquad+\frac{\partial \ln p_2}{\partial n_\lambda^{(2)}}\frac{dn_\lambda^{(2)}}{d\theta}-\frac{\partial \ln p_1}{\partial n_\lambda^{(1)}}\frac{dn_\lambda^{(1)}}{d\theta}+\frac{\partial \ln p_2}{\partial \ln \rho_2}\frac{d\ln M_2}{d\theta}-\frac{\partial \ln p_1}{\partial \ln \rho_1}\frac{d\ln M_1}{d\theta}
\end{aligned}\tag{I-78}$$

This equation simplifies considerably under two circumstances. The first arises if the composition of the gas is fixed, as would occur for the unburned gas. The second arises when the gas composition is in chemical equilibrium, as might happen for the burned gas. In both of these situations the pressure could be regarded as a function of internal energy and density alone. As a result the terms on the right side of the equation involving composition derivatives would be set to zero. Furthermore on the left side the combination of pressure derivatives is related to the isentropic exponent γ when the system is adiabatic.

$$\gamma \equiv \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_s = \frac{\partial \ln p}{\partial u}\left(\frac{\partial u}{\partial \ln \rho}\right)_s + \frac{\partial \ln p}{\partial \ln \rho}$$

But if we invoke the first law of thermodynamics

$$T\,ds = du + p\,d(1/\rho) = du - p\rho^{-1}\,d\ln\rho \tag{I-79}$$

for an isentropic process, it follows that

$$\left(\frac{\partial u}{\partial \ln \rho}\right)_s = p\rho^{-1}$$

and we immediately have the desired result

$$\gamma = p\rho^{-1}\frac{\partial \ln p}{\partial u} + \frac{\partial \ln p}{\partial \ln \rho} \tag{I-80}$$

I must mention that although the isentropic exponent is equal to the ratio of constant-pressure and constant-volume heat capacities for the fixed-composition case, this is not true when the composition is in chemical equilibrium. In practice, it is usually more convenient to treat the pressure as an explicit function of temperature rather than of internal energy. Since $c_v = \partial u/\partial T$, it is obvious that $\partial \ln p/\partial u = (Tc_v)^{-1}\,\partial \ln p/\partial \ln T$. Hence

$$\gamma = p\rho^{-1}\frac{\partial \ln p}{\partial u} + \frac{\partial \ln p}{\partial \ln \rho} = (\rho T c_v)^{-1} p\frac{\partial \ln p}{\partial \ln T} + \frac{\partial \ln p}{\partial \ln \rho} \tag{I-81}$$

and if the nonreacting gas obeys an ideal equation of state, this combination reduces to the heat capacity ratio.

Equation (I-78) is one relation connecting $dV_1/d\theta$ and $dV_2/d\theta$. A second equation is obtained by differentiation of the last member of equation (I-75).

$$\left(\frac{V_1}{V}\right)\frac{d\ln V_1}{d\theta} + \left(\frac{V_2}{V}\right)\frac{d\ln V_2}{d\theta} = \frac{d\ln V}{d\theta} \tag{I-82}$$

The volume fractions are easily related to the masses and densities.

$$\begin{aligned} \frac{V_1}{V} &= \frac{V_1}{V_1+V_2} = \left(1+\frac{V_2}{V_1}\right)^{-1} = \left(1+\frac{M_2\rho_1}{M_1\rho_2}\right)^{-1} \\ \frac{V_2}{V} &= 1 - \frac{V_1}{V} = \left(1+\frac{M_2\rho_1}{M_1\rho_2}\right)^{-1}\left(\frac{M_2\rho_1}{M_1\rho_2}\right) \end{aligned} \tag{I-83}$$

The pair of equations (I-78) and (I-82), supplemented by (I-80) or (I-81) where appropriate and (I-83), can be solved for $d\ln V_1/d\theta$ and $d\ln V_2/d\theta$.

Volume and area: The differential equations for the combustion and noncombustion phases will be solved for a prescribed variation of volume and surface area with crankangle. The form of this variation is easily obtained from the geometrical relationship depicted in figure 4 for the displacement of the piston $x(\theta)$ and can be expressed in terms of engine parameters l and r_0.

$$x(\theta) = l + r_0 - (l\cos\varphi + r_0\cos\theta) \tag{I-84}$$

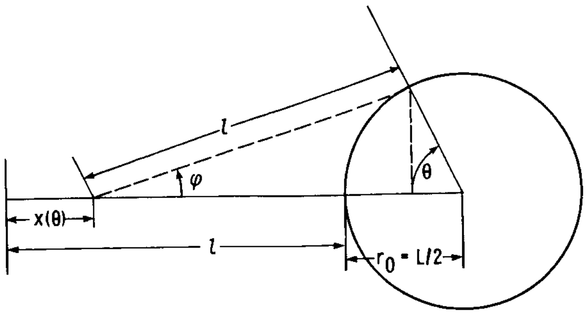


Figure 4. - Piston displacement geometry for crank-slider formula.

Geometrically it is clear that $l \sin \varphi = r_0 \sin \theta$ and hence $\cos^2\varphi = 1 - \sin^2\varphi = 1 - (r_0/l)^2 \sin^2\theta$. Consequently

$$\frac{2x(\theta)}{L} = 1 - \cos\theta + \epsilon^{-1}[1 - (1 - \epsilon^2 \sin^2\theta)^{1/2}] \tag{I-85}$$

where $\epsilon = L/2l$. Equation (I-85) is the usual crank-slider formula, and from this follows an equation for the volume.

$$V(\theta) = V(0) + \frac{\pi B^2}{4}\frac{L}{2}\left[\frac{2x(\theta)}{L}\right]$$

This formula for the volume is conveniently expressed in terms of the compression ratio $r = V(\pi)/V(0) = 1 + \pi B^2 L/4V(0)$.

$$V(\theta) = V(0)\left\{1 + (r-1)\frac{[1 - \cos\theta + (1 - \sqrt{1 - \epsilon^2 \sin^2\theta})/\epsilon]}{2}\right\} \tag{I-86}$$

Similarly the area dependence on crankangle can be expressed in terms of the compression ratio and engine parameters.

$$A(\theta) = A(0) + \frac{\pi BL}{2}\left[\frac{2x(\theta)}{L}\right] \tag{I-87}$$

But if we use

$$\pi BL = \left(\frac{\pi B^2 L}{4}\right)\left(\frac{4}{B}\right) = \frac{4[V(\pi) - V(0)]}{B} = \frac{4(r-1)V(0)}{B}$$

then

$$A(\theta) = A(0) + 2(r-1)V(0)\frac{[1 - \cos\theta + (1 - \sqrt{1 - \epsilon^2 \sin^2\theta})/\epsilon]}{B} \tag{I-88}$$

The minimum volume $V(0)$, the minimum area $A(0)$, the compression ratio r, the bore B, and the stroke L are engine parameters which must be specified to define the calculation.

Mass burning formulas: My choice for the mass burning rate function $\dot{M}_b$ is based on my analysis (ref. 42) of a burning model first proposed by Blizard and Keck (ref. 43). It is essentially a relaxation approach to burning, as can be easily seen from the governing differential equation.

$$\omega\tau\frac{dM_b}{d\theta}+M_b=M_f \tag{I-89}$$

If ignition begins at a crankangle θ_0 and the flame completely engulfs the working fluid over the crankangle interval $[\theta_0, \theta_f]$, then the general solution to this first-order equation can easily be written down for a prescribed function $M_f(\theta)$, the mass enveloped by the flame.

$$M_b(\theta)F(\theta)=M_b(\theta_0)+\int_{\theta_0}^{\theta} d\theta' \dot{F}(\theta')M_f(\theta') \tag{I-90}$$

The function $F(\theta)$ is defined by a quadrature

$$F(\theta)=\exp\left(\int_{\theta_0}^{\theta}\frac{d\theta'}{\omega\tau}\right) \tag{I-91}$$

and $\dot{F}(\theta)$ is its derivative with respect to θ.

The choice of M_f is not wholly arbitrary because on physical grounds M_f must be a nondecreasing function of θ, that is, $\dot{M}_f \geq 0$. But the nondecreasing nature of M_f is adequate to establish that the resulting M_b is also nondecreasing as required in equation (I-74). It is easily seen from the differential equation (I-89) that for $\omega\tau=0$ we have $M_b=M_f$ and hence $\dot{M}_b \geq 0$ if and only if $\dot{M}_f \geq 0$. When $\omega\tau > 0$, the differential equation (I-89) shows that $\dot{M}_b \geq 0$ if and only if $M_b - M_f \leq 0$, and an integration by parts in equation (I-90) establishes an expression for $M_b - M_f$.

$$[M_b(\theta)-M_f(\theta)]F(\theta)=M_b(\theta_0)-M_f(\theta_0)-\int_{\theta_0}^{\theta} d\theta' F(\theta')\dot{M}_f(\theta')$$

But $F(\theta)>0$ for all $\theta \geq \theta_0$ and thus $\dot{M}_f \geq 0$ and $M_b(\theta_0)-M_f(\theta_0) \leq 0$ imply $M_b(\theta)-M_f(\theta) \leq 0$ for all θ, which establishes $\dot{M}_b \geq 0$.

Two broad classes of functions will be considered for the function M_f. The first class, referred to as Fourier burning functions, are of the form

$$M_f=\begin{cases} M_b(\theta_0)+[M(\theta_0)-M_b(\theta_0)]\sum\limits_{n=0}^{\infty} a_n \cos n\pi z & \theta_0 \leq \theta \leq \theta_f \\ M(\theta_0) & \theta_f < \theta \end{cases} \tag{I-92}$$

where $z=(\theta-\theta_0)/(\theta_f-\theta_0)$. The name simply refers to the fact that this is nothing more than a Fourier cosine expansion of M_f, which in practice will be truncated to a finite number of terms. The expansion coefficients a_n are restricted by the conditions that $M_f(\theta_0)=M_b(\theta_0)$ and $M_f(\theta_f)=M(\theta_0)$. These lead to the requirements

$$\sum_{n=0}^{\infty} a_n = 0$$

$$\sum_{n=0}^{\infty} a_n(-1)^n = 1$$

and can be expressed as separate conditions on the even and odd coefficients.

$$\sum_{n=0}^{\infty} a_{2n} = 1/2$$

$$\sum_{n=0}^{\infty} a_{2n+1} = -1/2 \tag{I–93}$$

The condition $\dot{M}_f \geq 0$ places another constraint on the expansion coefficients.

$$\sum_{n=1}^{\infty} n a_n \sin n\pi z \leq 0 \tag{I–94}$$

This can be translated into conditions on the expansion coefficients for the special case where $a_n = 0$ for $n \geq 4$. Then it can be written as

$$a_1 \sin \pi z + 2a_2 \sin 2\pi z + 3a_3 \sin 3\pi z = (\sin \pi z)\{a_1 + 4a_2 \cos \pi z + 3a_3[3 - 4(1 - \cos^2 \pi z)]\} \leq 0$$

by using trigonometric identities for the sine of twice and three times the angle πz. Since $0 \leq z \leq 1$, $\sin \pi z$ is always positive and vanishes only at the ends of the interval. Consequently we are left with the condition

$$a_1 - 3a_3 + 4a_2 \cos \pi z + 12a_3 \cos^2 \pi z \leq 0 \tag{I–95}$$

Examination of the behavior of this quadratic function of $\cos \pi z$ over the interval $-1 \leq \cos \pi z \leq 1$ leads to conditions on a_1, a_2, and a_3 for various conditions.

$-1/8 \leq a_3 \leq 1/16 + \min\{a_2, -a_2\}/2$

If $a_3 = 0$, then $|a_2| \leq -a_1/4 = 1/8$

If $a_2 < -6|a_3|$ and $a_3 \neq 0$, then $a_1 + 9a_3 - 4a_2 \leq 0$

If $a_2 > 6|a_3|$ and $a_3 \neq 0$, then $a_1 + 9a_3 + 4a_2 \leq 0$ (I–96)

If $-6|a_3| \leq a_2 \leq 6|a_3|$ and $a_3 > 0$, then $\max\{a_1 + 9a_3 - 4a_2,\ a_1 + 9a_3 + 4a_2\} \leq 0$

If $-6|a_3| \leq a_2 \leq 6|a_3|$ and $a_3 < 0$, then $a_1 - 3a_3 - (a_2)^2/3a_3 \leq 0$

Substituting the expression (I–92) for M_f into the general solution (I–90) and assuming $\omega\tau$ to be independent of θ give a simple expression for M_b and its derivative $\dot{M}_b$.

$$M_b = \begin{cases} M_b(\theta_0) + [M(\theta_0) - M_b(\theta_0)] \sum_{n=0}^{\infty} a_n \left[\dfrac{\cos n\pi z + \lambda n \sin n\pi z - e^{-\pi z/\lambda}}{1 + (\lambda n)^2} \right] & \theta_0 \le \theta \le \theta_f \\ M_b(\theta_f) + [M(\theta_0) - M_b(\theta_f)]\{1 - \mathrm{e}^{-(\theta - \theta_f)/\omega\tau}\} & \theta_f < \theta \end{cases}$$

$$\dot{M}_b = \begin{cases} \dfrac{[M(\theta_0) - M_b(\theta_0)]}{\omega\tau} \sum_{n=0}^{\infty} a_n \left[\dfrac{-\lambda n \sin n\pi z + (\lambda n)^2 \cos n\pi z + e^{-\pi z/\lambda}}{1 + (\lambda n)^2} \right] & \theta_0 \le \theta \le \theta_f \\ \dfrac{[M(\theta_0) - M_b(\theta_f)]}{\omega\tau} e^{-(\theta - \theta_f)/\omega\tau} & \theta_f < \theta \end{cases} \tag{I-97}$$

The parameter λ is defined by $\lambda = \pi\omega\tau/(\theta_f - \theta_0)$. When $\omega\tau = 0$, we have $M_b = M_f$ and consequently $\dot{M}_b = \dot{M}_f$.

$$\dot{M}_b = \begin{cases} \dfrac{-\pi[M(\theta) - M_b(\theta_0)]}{\theta_f - \theta_0} \sum_{n=1}^{\infty} n a_n \sin n\pi z & \theta_0 \le \theta \le \theta_f \\ 0 & \theta_f < \theta \end{cases} \qquad \omega\tau = 0 \tag{I-98}$$

The special choice $a_0 = 1/2$, $a_1 = -1/2$, and $a_n = 0$ for $n = 2, 3, \ldots$ gives the cosine burning function used by Blumberg and Kummer (ref. 23) for the case $\omega\tau = 0$. The addition of just one other parameter, a_2 or a_3, enhances the flexibility of M_f considerably. From equations (I-93) and (I-96) we have that for $a_3 = 0$, $|a_2| \le 1/8$, while for $a_2 = 0$ we find that $-1/8 \le a_3 \le 1/16$. The behavior of M_f for the two extremes of parameter values as well as for the Blumberg-Kummer M_f are shown in figure 5. Increasing a_2 tends to displace M_f to higher values of θ, while decreasing a_3 tends to rotate M_f nonuniformly in a clockwise direction about its midpoint. The value of M_f at the midpoint of the z interval is determined by $a_0 - a_2$ in the four-parameter version of M_f.

The second class of functions used for M_f is a two-parameter family with the structure

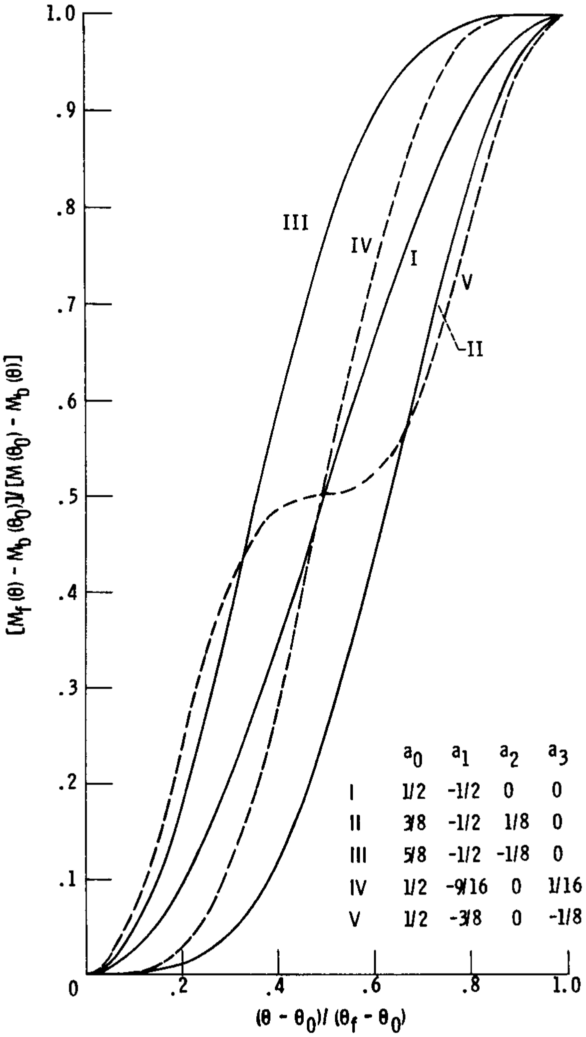
$$M_f = \begin{cases} M_b(\theta_0) + [M(\theta_0) - M_b(\theta_0)][1 + e^{-\alpha z^\beta}(z^{\beta - 1} - 1)] & \theta_0 \le \theta \le \theta_f \\ M(\theta_0) & \theta_f < \theta \end{cases} \tag{I-99}$$

with the two parameters α and β presumed to be independent of θ. If α and β are constrained to satisfy the condition

$$\alpha\beta = \frac{(\theta_f - \theta_0)}{\omega\tau} > 0 \tag{I-100}$$

then it can be verified that

$$M_b = \begin{cases} M_b(\theta_0) + [M(\theta_0) - M_b(\theta_0)][1 - e^{-\alpha z^\beta}] & \theta_0 \le \theta \le \theta_f \\ M_b(\theta_f) + [M(\theta_0) - M_b(\theta_f)]\{1 - \mathrm{e}^{-(\theta - \theta_f)/\omega\tau}\} & \theta_f < \theta \end{cases} \tag{I-101}$$



	a_0	a_1	a_2	a_3
I	1/2	-1/2	0	0
II	3/8	-1/2	1/8	0
III	5/8	-1/2	-1/8	0
IV	1/2	-9/16	0	1/16
V	1/2	-3/8	0	-1/8

Figure 5. - Examples of Fourier burning formula.

and M_f as given in equation (I-99) satisfy the differential equation (I-89). The expression for M_b in the interval $\theta_0 \leq \theta \leq \theta_f$ coincides with the burning function introduced by Wiebe (ref. 44) and used recently by Tabacyznski and Klomp (ref. 45). The derivative of equation (I-101) has a very simple form.

$$\dot{M}_b = \begin{cases} \dfrac{[M(\theta_0) - M_b(\theta_0)]}{\omega\tau} z^{\beta - 1} e^{-\alpha z^\beta} & \theta_0 \leq \theta \leq \theta_f \\[2ex] \dfrac{[M(\theta_0) - M_b(\theta_f)]}{\omega\tau} e^{-(\theta - \theta_f)/\omega\tau} & \theta_f < \theta \end{cases} \qquad \text{(I-102)}$$

The product $\alpha\beta$ is positive as indicated by equation (I-100). But to assure that M_b takes an appropriate value at $z = 0$, it is necessary to require that β be positive, and consequently, α also must be positive.

The function (I-99) contains a degenerate case, in the sense of violating equation (I-100), corresponding to $\alpha = 0$. In particular if $\beta = 2$ and $\alpha = 0$, we obtain the linear burning expression

$$M_f = \begin{cases} M_b(\theta_0) + [M(\theta_0) - M_b(\theta_0)]z & \theta_0 \le \theta \le \theta_f \\ M(\theta_0) & \theta_f < \theta \end{cases} \qquad \text{(I-103)}$$

This gives an extremely simple expression for M_b and $\dot{M}_b$

$$M_b = \begin{cases} M_b(\theta_0) + [M(\theta_0) - M_b(\theta_0)]\left[z - \frac{\omega\tau}{(\theta_f - \theta_0)}\left(1 - e^{-(\theta-\theta_0)/\omega\tau}\right)\right] & \theta_0 \le \theta \le \theta_f \\ M_b(\theta_f) + [M(\theta_0) - M_b(\theta_f)](1 - \mathrm{e}^{-(\theta-\theta_f)/\omega\tau}) & \theta_f < \theta \end{cases}$$

$$\text{(I-104)}$$

$$\dot{M}_b = \begin{cases} \frac{[M(\theta_0) - M_b(\theta_0)]}{\theta_f - \theta_0}\left[1 - e^{-(\theta-\theta_0)/\omega\tau}\right] & \theta_0 \le \theta \le \theta_f \\ \frac{[M(\theta_0) - M_b(\theta_f)]}{\omega\tau} e^{-(\theta-\theta_f)/\omega\tau} & \theta_f < \theta \end{cases}$$

Heat transfer coefficients: At the present time there is considerable uncertainty about an appropriate expression for the heat transfer coefficient in an internal combustion engine. This situation arose from two principal factors. The first was, and is, the relative paucity of good, published, experimental data on the heat loss from an engine. The second was the inability to carry out sufficiently detailed model cycle calculations to permit a comparison of experiment and calculation with a view toward extraction of heat transfer parameters from the comparison. This has not deterred people from proposing many different expressions for the heat transfer coefficient. Annand (ref. 46) reviewed eight such formulas proposed before 1963, found all of them wanting, and suggested his own version. Subsequently Woschni (ref. 47) gave still another formula. Of all of the suggested formulas the one propounded by Eichelberg (ref. 48) is probably the most widely used.

I have chosen to calculate the heat transfer coefficient from a formula that is sufficiently general to encompass a number of the suggested forms.

$$\bar{h} = c_1 + c_2\left(\frac{k}{B}\right)(\mathrm{Pr})^a(\mathrm{Re})^b + c_3\frac{T^4 - T_w^4}{T - T_w} + c_4 v^{1/3}(pT)^{1/2} \qquad \text{(I-105)}$$

The Prandtl number is defined in terms of the constant-pressure specific heat, viscosity, and thermal conductivity by the formula

$$\mathrm{Pr} = \frac{c_p \eta}{k} \qquad \text{(I-106)}$$

and the Reynolds number is defined as

$$\mathrm{Re} = \frac{Dv\rho}{\eta} \qquad \text{(I-107)}$$

The velocity v is obtained from the expression

$$v = b_1 v_m + (1 - b_1) v_p + \frac{b_2 \omega}{M(\theta)} \frac{dM_b}{d\theta} \tag{I-108}$$

where D is a length usually set to the bore B, b_1 is a dimensionless parameter, and b_2 is a parameter with the dimension of length. When $b_2 = 0$ and $b_1 = 1$, the velocity is the mean piston speed $v_m = L\omega/\pi$, while for $b_2 = 0 = b_1$ it is the piston speed whose value can be calculated from the derivative of equation (I-85) with respect to time.

$$v_p = \frac{\pi}{2} v_m \left| \sin\theta \left[1 + \epsilon (1 - \epsilon^2 \sin^2\theta)^{-1/2} \cos\theta \right] \right| \tag{I-109}$$

The last term in equation (I-108) attempts to account for augmentation of heat transfer by combustion. Such an effect was suggested by Woschni, who used the pressure difference between the fired and motored engine to characterize the phenomenon. This approach is computationally and philosophically unsatisfactory for its implementation requires a knowledge of the motored behavior and implies that the fired engine must somehow base its response on its motored behavior rather than on its current condition. The choices $c_2 = c_3 = c_4 = 0$ made in equation (I-105) give a constant heat transfer coefficient, while the choices $c_1 = c_2 = c_3 = 0$ give the Eichelberg form for the heat transfer coefficient. The Annand heat transfer coefficient corresponds to $c_1 = c_4 = a = 0$ with $v = v_m$ and $D = B$. The well-known Dittus-Boelter correlation for heat transfer accompanying turbulent flow in a pipe is obtained for $c_1 = c_3 = c_4 = 0$. Karim and Watson's (ref. 49) expression for $\bar{h}$ corresponds to $c_1 = c_3 = c_4 = a = 0$ with D equal to the piston-to-head distance and $v = v_p$.

Intake and exhaust flow: The equations for $\dot{M}^{(\pm)}$ are based on the form suggested by equations (I-70) and (I-71). Suppose that the subscript 1 refers to "upstream" conditions and 2 refers to "downstream" conditions in the sense that $p_2 \leq p_1$. Then for $\gamma_1 \neq 1$

$$\left|\dot{M}^{(\pm)}\right| = \begin{cases} \dfrac{\rho_1 A^{(\pm)}}{\omega} \left\{ \dfrac{2 p_1 \rho_1^{-1} \gamma_1 (\gamma_1 - 1)^{-1} \left[\sigma(\pm) - (p_2/p_1)^{(\gamma_1 - 1)/\gamma_1} \right]}{(p_1/p_2)^{2/\gamma_1} - b^{(\pm)}} \right\}^{1/2} & p_2/p_1 > (p_2/p_1)_c \\ \dfrac{\rho_1 A^{(\pm)}}{\omega} \left\{ \dfrac{2 p_1 \rho_1^{-1} \gamma_1 (\gamma_1 - 1)^{-1} \left[\sigma(\pm) - (p_2/p_1)_c^{(\gamma_1 - 1)/\gamma_1} \right]}{(p_1/p_2)_c^{2/\gamma_1} - b^{(\pm)}} \right\}^{1/2} & (p_2/p_1) \leq (p_2/p_1)_c \end{cases} \tag{I-110}$$

where

$$\sigma(\pm) = 1 + \frac{e^{(\pm)} (\gamma_1 - 1)}{\gamma_1 p_1 \rho_1^{-1}} \tag{I-111}$$

while for $\gamma_1 = 1$

$$\left|\dot{M}^{(\pm)}\right| = \begin{cases} \dfrac{\rho_1 A^{(\pm)}}{\omega} \left\{ \dfrac{2 p_1 \rho_1^{-1} \left[\sigma(\pm) + \ln(p_1/p_2) \right]}{(p_1/p_2)^2 - b^{(\pm)}} \right\}^{1/2} & p_2/p_1 > (p_2/p_1)_c \\ \dfrac{\rho_1 A^{(\pm)}}{\omega} \left\{ \dfrac{2 p_1 \rho_1^{-1} \left[\sigma(\pm) + \ln(p_1/p_2)_c \right]}{(p_1/p_2)_c^2 - b^{(\pm)}} \right\}^{1/2} & p_2/p_1 \leq (p_2/p_1)_c \end{cases} \tag{I-112}$$

where

$$\sigma(\pm) = \frac{e^{(\pm)}}{p_1 \rho_1^{-1}} \tag{I-113}$$

The direction of flow is always from the higher to the lower pressure, with $\dot{M}^{(\pm)}$ chosen as positive when the flow is into the cylinder. As a result we can express the mass flow rates for the intake and exhaust systems as

$$\begin{aligned} \dot{M}^{(+)} &= |\dot{M}^{(+)}|\operatorname{sgn}(p_m - p) \\ \dot{M}^{(-)} &= |\dot{M}^{(-)}|\operatorname{sgn}(p_e - p) \end{aligned} \tag{I-114}$$

where p_m is the inlet manifold pressure, p_e the exhaust system pressure, and p the pressure in the cylinder. The critical pressure ratio $(p_2/p_1)_c$ is the value of the pressure ratio for which $|\dot{M}^{(\pm)}|$ attains its maximum value. Its value can be calculated as the solution of

$$\begin{aligned} &2\sigma^{(\pm)} - (\gamma_1 + 1)\left(\frac{p_2}{p_1}\right)_c^{(\gamma_1-1)/\gamma_1} + b^{(\pm)}(\gamma_1 - 1)\left(\frac{p_2}{p_1}\right)_c^{(\gamma_1+1)/\gamma_1} = 0 \qquad \gamma_1 \neq 1 \\ &1 - 2\sigma^{(\pm)} - b^{(\pm)}\left(\frac{p_2}{p_1}\right)_c^2 + 2\ln\left(\frac{p_2}{p_1}\right)_c = 0 \qquad \gamma_1 = 1 \end{aligned} \tag{I-115}$$

where equation (I-115) is obtained by setting to zero the derivative of $|\dot{M}^{(\pm)}|$ with respect to p_2/p_1 and canceling all nonzero factors in the expression for the derivative. The values of $A^{(\pm)}$ with dimensions of length squared, $e^{(\pm)}$ with dimensions of energy per unit mass, and $b^{(\pm)}$, which is dimensionless, may be explicit or implicit functions of crankangle but not of pressure ratio. Since $|\dot{M}^{(\pm)}| \geq 0$, then $A^{(\pm)} \geq 0$ and, because $|\dot{M}^{(\pm)}|$ must be real, $\sigma^{(\pm)}$ and $b^{(\pm)}$ must be such that the argument of the square root in equations (I-110) and (I-112) is nonnegative. The equations for $|\dot{M}^{(\pm)}|$ reduce to the conventionally used equations when $e^{(\pm)} = 0 = b^{(\pm)}$ and $A^{(\pm)}$ equals an area multiplied by a discharge coefficient.

Just as there is an uncertainty about a suitable expression for the heat transfer coefficient, so too there is an uncertainty about the correct forms for the functions $A^{(\pm)}$, $e^{(\pm)}$, and $b^{(\pm)}$. Clearly these quantities must reflect the geometrical and fluid mechanical realities of the poppet valves used in internal combustion engines. The experimental studies by Woods and Khan (ref. 50) and Woods (ref. 51) on single and twin poppet valves, respectively, at least point to tentative choices for $A^{(\pm)}$, $e^{(\pm)}$, and $b^{(\pm)}$. They investigated both normal and reverse flows through poppet valves as a function of valve lift, pressure ratio across the valve, and wall proximity. The experimental results were expressed as a dimensionless, effective, cross-sectional area for flow A^*_{eff}. Their definition of A^*_{eff} can be expressed relatively simply in terms of $A^{(\pm)}$, $\sigma^{(\pm)}$ and $b^{(\pm)}$ by using equation (I-110).

$$\begin{aligned} A^*_{\text{eff}} &\equiv \frac{|\dot{M}^{(\pm)}|\omega(p_2/p_1)^{-1/\gamma_1}}{\rho_1[\pi(d^{(\pm)2})/4]}\left\{2p_1\rho_1^{-1}\gamma_1(\gamma_1-1)^{-1}\left[1-\left(\frac{p_2}{p_1}\right)^{(\gamma_1-1)/\gamma_1}\right]\right\}^{-1/2} \\ &= \left[\frac{A^{(\pm)}}{\pi(d^{(\pm)2})/4}\right]\left\{\left[\sigma^{(\pm)} - \left(\frac{p_2}{p_1}\right)^{\gamma_1/(\gamma_1-1)-1}\right]\right. \\ &\qquad \left.\times\left[1-\left(\frac{p_2}{p_1}\right)^{\gamma_1/(\gamma_1-1)}\right]^{-1}\left[1-b^{(\pm)}\left(\frac{p_2}{p_1}\right)^{2/\gamma_1}\right]^{-1}\right\}^{1/2} \end{aligned}$$

The geometrical situation, illustrated in figure 6, is governed by such factors as valve lift, valve seat angle, valve diameter, valve thickness, and a variable which we do not consider explicity, wall

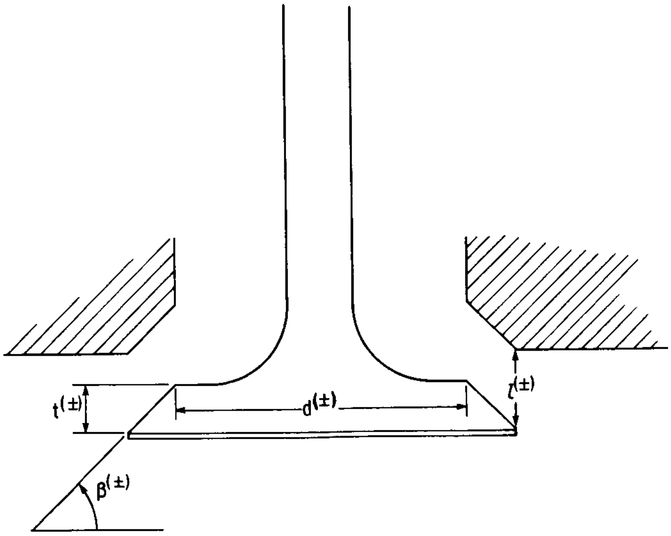


Figure 6. - Poppet valve geometry.

proximity. The actual cross-sectional flow area is calculable from these and, relative to the minimum cross-sectional area of the valve $\pi(d^{(\pm)})^2/4$, is given by $4(l^{(\pm)}/d^{(\pm)})\cos\beta^{(\pm)}$ to first order in $l^{(\pm)}/d^{(\pm)}$. Actually since the flow area can be viewed as the surface of the frustum of a right cone, the exact expression is given by

$$\frac{4A_{\text{flow}}^{(\pm)}}{\pi d^{(\pm)2}} = 4\frac{l^{(\pm)}}{d^{(\pm)}}\cos\beta^{(\pm)}[1+\alpha^{(\pm)}(l^{(\pm)}/d^{(\pm)})] \tag{I-116a}$$

where

$$\alpha^{(\pm)} = \frac{2\cos^2\beta^{(\pm)}}{\tan\beta^{(\pm)}} + \frac{1}{2}\sin 2\beta^{(\pm)} \tag{I-116b}$$

Strictly speaking, the expression for $A_{\text{flow}}^{(\pm)}$ is valid only so long as $l^{(\pm)}\cos^2\beta^{(\pm)} \leq t^{(\pm)}$. Suppose that the fluid mechanical behavior can be characterized by a Reynolds number $\text{Re}^{(\pm)}$. It is convenient to base the Reynolds number on the valve lift, a mass flux calculated from $|\dot{M}^{(\pm)}|$, and the actual cross-sectional area. This leads to the Reynolds number

$$\text{Re}^{(\pm)} = \frac{l^{(\pm)}|\dot{M}^{(\pm)}|\omega}{\eta A_{\text{flow}}^{(\pm)}} = \frac{|\dot{M}^{(\pm)}|\omega}{\pi d^{(\pm)}\eta\cos\beta^{(\pm)}}[1+\alpha^{(\pm)}(l^{(\pm)}/d^{(\pm)})]^{-1} \tag{I-116c}$$

which is dependent on valve lift. The first factor corresponds exactly to the form of the Reynolds number used by Whitehouse et al. (ref. 15). The value of $\text{Re}^{(\pm)}$ can be expected to be about 10^6 or less under typical conditions. The experimental results were shown as a parametric family of curves of A_{eff}^{*} versus $l^{(\pm)}/d^{(\pm)}$ with p_1/p_2 as the labeling parameter. But for a fixed geometrical situation, $|\dot{M}^{(\pm)}|$ increases monotonically with p_1/p_2 and consequently so too does $Re^{(\pm)}$. Under these circumstances p_1/p_2 can be replaced by $Re^{(\pm)}$ as a parameter without altering the nature of the curves for A_{eff}^{*}. With this understanding we can interpret the experimental results for A_{eff}^{*}. For small $l^{(\pm)}/d^{(\pm)}$ (<0.1), all curves coalesce to a single linear curve with a slope of 2.6. This value is very close to $4\cos\beta^{(\pm)} = 2.8$ for $\beta^{(\pm)} = \pi/4$, which corresponds to the valve seat angle used in the experiments. In fact, less than a 4° increase in $\beta^{(\pm)}$ is all that is necessary to get full agreement with 2.6. This suggests that for small $l^{(\pm)}/d^{(\pm)}$ the area $A^{(\pm)}$ is in fact the actual flow area. For larger values of $l^{(\pm)}/d^{(\pm)}$ the experimental A_{eff}^{*} falls below the extrapolation of the initial slope and becomes dependent on the Reynolds number with A_{eff}^{*} increasing with $Re^{(\pm)}$ for a fixed $l^{(\pm)}/d^{(\pm)}$.

The general appearance of A^{*}_{eff} seems to be that of a function quadratic in $l^{(\pm)}/d^{(\pm)}$ with a maximum somewhere near the maximum value of $l^{(\pm)}/d^{(\pm)}$. If all of the dependence on valve lift is ascribed to $A^{(\pm)}$, then $e^{(\pm)}$ and $b^{(\pm)}$ will depend only on $Re^{(\pm)}$. In light of these observations I shall write expressions for $A^{(\pm)}$, $e^{(\pm)}$, and $b^{(\pm)}$ which seem adequate for the representation of the experimental observations.

$$\frac{A^{(\pm)}}{\pi(d^{(\pm)})^2/4} = \frac{4A^{(\pm)}_{\text{flow}}}{\pi(d^{(\pm)})^2}\left(1-\frac{l^{(\pm)}}{2l_0^{(\pm)}}\right)\left[A_1^{(\pm)}+A_2^{(\pm)}(Re^{(\pm)}\times 10^{-6})^{A_3^{(\pm)}}\right]$$

$$\frac{\rho_1 e^{(\pm)}}{p_1} = \left[E_1^{(\pm)}+E_2^{(\pm)}(Re^{(\pm)}\times 10^{-6})^{E_3^{(\pm)}}\right]\,(Re^{(\pm)}\times 10^{-6})^{E_4^{(\pm)}} \qquad \text{(I-117a)}$$

$$b^{(\pm)} = b_1^{(\pm)}+b_2^{(\pm)}(Re^{(\pm)}\times 10^{-6})^{b_3^{(\pm)}}$$

In evaluating of the right side of equation (I-117a) the assumption is made that $A_3^{(\pm)}=0$ implies $A_2^{(\pm)}=0$, that $E_3^{(\pm)}=0$ implies $E_2^{(\pm)}=0$, and that $b_3^{(\pm)}=0$ implies $b_2^{(\pm)}=0$. I assume that the parameters $l_0^{(\pm)}$, $A_k^{(\pm)}$, $E_k^{(\pm)}$, and $b_k^{(\pm)}$ can depend only on the sign of $\dot{M}^{(\pm)}$, that is, they are constants whose values depend solely on the direction of flow. Furthermore, since it is physically necessary that $p_2/p_1=1$ implies $\dot{M}^{(\pm)}=0$, the constants $E_k^{(\pm)}$ must be chosen so that $e^{(\pm)}=0$ when $Re^{(\pm)}=0$. The factor 10^{-6} is included with $Re^{(\pm)}$ for scaling purposes. The valve lift $l^{(\pm)}$ is an explicit function of crankangle taken as

$$\frac{l^{(\pm)}}{d^{(\pm)}} = P^{(\pm)}(x^{(\pm)}) \qquad x^{(\pm)} = \left(\theta-\theta_c^{(\pm)}\right)\Big/\left(\theta_o^{(\pm)}-\theta_c^{(\pm)}\right)$$

$$P(x) = \begin{cases} \displaystyle\sum_{n=1}^{10} r_n x^n, \quad \sum_{n=1}^{10} r_n = 0 & \text{(polynomial form)} \\ \displaystyle x(1-x)\exp\left(\sum_{n=1}^{10} r_n x^{n-1}\right) & \text{(exponential form)} \end{cases} \qquad \text{(I-117b)}$$

where the r_n are constants which must be determined by fitting experimental data.

The capability of the functions (I-117) to generate an A^{*}_{eff} function similar to what is obtained from experimental measurements is shown in figure 7. The curves were calculated for air at an upstream pressure of 1 atmosphere and a temperature of 298.15 K. The viscosity was approximated as 1.7×10^{-4} poise and the first order approximation to the flow area was used ($\alpha^{(\pm)}=0$).

While equations (I-110) to (I-117) do completely define $\dot{M}^{(\pm)}$ during a cycle, they do not completely determine $M^{(+)}$ and $M^{(-)}$, which still contain arbitrary constants of integration. The definition is completed by specifying a value for each function at some point in the cycle. Suppose $\theta_o^{(\pm)}$ and $\theta_c^{(\pm)}$ are the crankangle values for valve openings and closings, respectively. It is convenient to complete the definition of $M^{(-)}$ by choosing $M^{(-)}(\theta_o^{(-)})=0$ for this makes $M^{(-)}$ continuous over the cycle except at the point $\theta_o^{(-)}$, where it experiences a discontinuous change from a negative value to zero. For the intake system it is convenient to position the discontinuity in $M^{(+)}$ at the point where it achieves its maximum value. This will occur at or slightly before $\theta_c^{(+)}$. Such a choice assures us that $M^{(+)}\leq 0$ prior to intake valve opening and virtually guarantees that $M^{(+)}$ will change sign only once during a cycle for reasonable choices of $\theta_o^{(+)}$ and $\theta_c^{(+)}$. This difference in location of the discontinuities reflects the differing roles of the intake and exhaust systems. A sketch of $\dot{M}^{(\pm)}$ and $M^{(\pm)}$ is given in figure 8. As defined here, both $M^{(+)}$ and $M^{(-)}$ are nonpositive at the start of a cycle ($\theta=4\pi n$, $n=0, 1, 2, \ldots$).

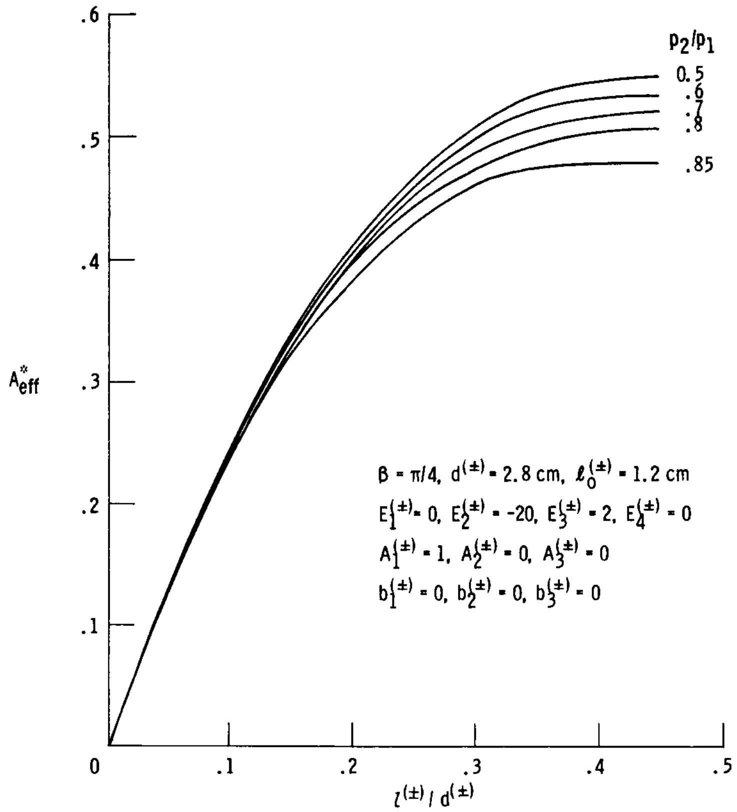


Figure 7. - Dimensionless effective area for flow of air through a poppet valve.

To complete the characterization of the flow, it is still necessary to specify how the state of the fluid changes as it flows from the upstream side to the downstream side. I shall assume that the composition is unchanged as the gas flows through the intake or exhaust system; however, the thermodynamic variables will be permitted to change in one of two possible modes. The two processes are, in a sense, representative of the extremes of all flow processes. The first possibility is that the flow is isentropic. From the first law of thermodynamics (eq. (I-79)) it follows that for such a process the change in internal energy is

$$u_2 - u_1 = -\int_{\rho_1}^{\rho_2} p \, d(1/\rho)$$

and corresponds to a maximum consumption of internal energy during the flow because the pressure opposing the flow is always the local gas pressure. For the second possibility we assume that a smaller amount of internal energy is expended during the flow, an amount equal to that calculated when p in the integrand is replaced by the constant downstream pressure p_2, which is always less than or equal to the local pressure. That is, the second type of flow is characterized by the condition

$$u_2 - u_1 = -p_2\left(\rho_2^{-1} - \rho_1^{-1}\right)$$

which can be written in an equivalent form.

$$h_2 = h_1 + \frac{p_2 - p_1}{\rho_1}$$

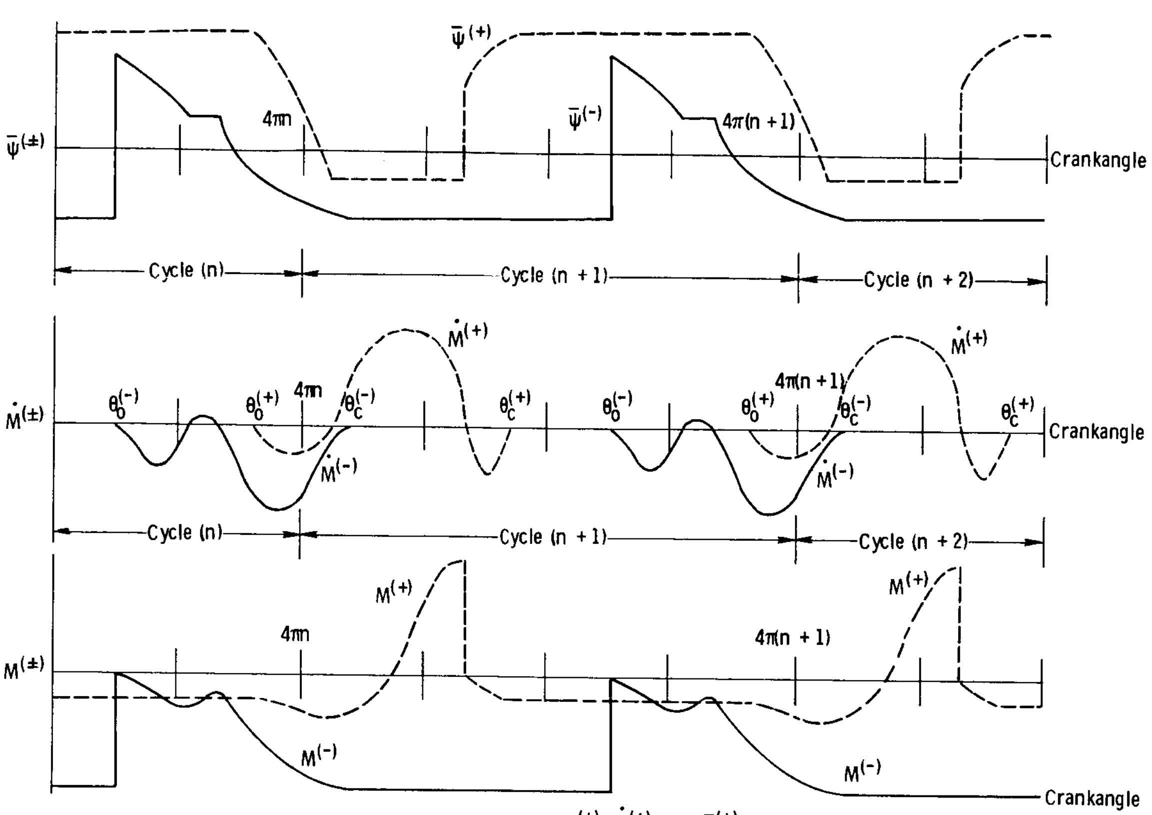


Figure 8. - Sketch of typical behavior of $M^{(\pm)}$, $\dot{M}^{(\pm)}$, and $\bar{\psi}^{(\pm)}$ as function of crankangle.

The thermodynamic changes associated with the two types of flows can be summarized by relating the lower pressure (downstream) state to the higher pressure (upstream) state.

Initial state	Final state
$n_\lambda(1)$, s_1, p_1, h_1	$n_\lambda(2)=n_\lambda(1)$, p_2, $s_2=s_1$ (isentropic process)
	$n_\lambda(2)=n_\lambda(1)$, p_2, $h_2=h_1+(p_2-p_1)/\rho_1$ (minimum u change process)

(I-118)

Now that $M^{(\pm)}$, $\dot{M}^{(\pm)}$, and the change of state accompanying flow have been defined, it will be convenient to define for later use a function of crankangle which serves as a measure of some average property for material which has emanated from the cylinder to that point in the cycle. We shall separately need such averages for the exhaust system and the intake system. Since some of the material leaving at one point in the cycle may return at a subsequent point, we need an average which is representative of the net efflux through the intake or exhaust system. Suppose U is a characteristic function defined as

$$U(x) = \begin{cases} 1 & x<0 \\ 0 & x\geq 0 \end{cases} \tag{I-119}$$

and $\psi = \psi(\theta)$ represents some property per unit mass associated with the effluent stream, such as enthalpy or moles of species. Furthermore define the nodes of $\dot{M}^{(\pm)}$ as those points for which $\dot{M}^{(\pm)} = 0$ and for which the value of $\dot{M}^{(\pm)}$ changes sign as the point is crossed. Label the nodes sequentially by $\theta_k^{(\pm)}$, $k = 1, 2, \ldots$, such that $\theta_1^{(\pm)}$ coincides with a discontinuity in $M^{(\pm)}$. Then the average $\bar{\psi}(\theta)^{(\pm)}$ is defined sequentially as the crankangle increases beyond $\theta_1^{(\pm)}$.

$$\bar{\psi}(\theta)^{(\pm)} = \begin{cases} 0 \qquad \text{at discontinuities in } M^{(\pm)} \\[2ex] \dfrac{M^{(\pm)}\left(\theta_k^{(\pm)}\right)\bar{\psi}^{(\pm)}\left(\theta_k^{(\pm)}\right)U\left[M^{(\pm)}\left(\theta_k^{(\pm)}\right)\right] + \int_{\theta_k^{(\pm)}}^{\theta} \psi(\theta')\dot{M}^{(\pm)}(\theta')U\left[\dot{M}^{(\pm)}(\theta')\right]\,d\theta'}{M^{(\pm)}\left(\theta_k^{(\pm)}\right)U\left[M^{(\pm)}\left(\theta_k^{(\pm)}\right)\right] + \int_{\theta_k^{(\pm)}}^{\theta} \dot{M}^{(\pm)}(\theta')U\left[\dot{M}^{(\pm)}(\theta')\right]\,d\theta'} \\[2ex] \qquad \theta_k^{(\pm)} < \theta \le \theta_{k+2}^{(\pm)} \qquad k = 1, 3, 5, \ldots \end{cases} \tag{I-120}$$

A couple of observations about this function should be made. First, $\bar{\psi}^{(\pm)}$ is reset to zero at all discontinuities in $M^{(\pm)}$. Second, the value of $\bar{\psi}^{(\pm)}$ remains constant over those crankangle regions where $\dot{M}^{(\pm)} \ge 0$ because the integrands vanish there. This definition defines $\bar{\psi}^{(\pm)}$ from one discontinuity of $M^{(\pm)}$ to the next. The value $\bar{\psi}^{(-)}(\theta_c^{(-)})$ represents the mass-averaged value of ψ contained in the exhaust. A sketch of $\bar{\psi}^{(\pm)}$ is shown as a part of figure 8. Naturally if ψ were a nonnegative property, then $\bar{\psi}^{(\pm)}$ would also be nonnegative.

Mixing of flow streams: During a cycle calculation it is sometimes necessary to mix two or more streams externally to the cylinder. Examples of the formation of such mixtures are the mixing of the reactants, typically hydrocarbon fuels and air, at their ambient conditions, and the mixing of these reactants with recirculated exhaust gases to form the fresh charge for the cylinder. Even the formation of the composite exhaust gas, which represents the average of the exhaust gas over a cycle, can be regarded as such a mixing process. In all such cases we need to know the state of the mixture for subsequent use in calculations or as a measure of the operation of the engine. I shall assume the mixing process to be a constant-pressure process unaccompanied by chemical reaction. If the streams to be mixed are initially at different pressures, then they can be separately brought to the mixing pressure by one of the two thermodynamic processes shown schematically as equation (I-118). The state of the mixture is defined by the mixing pressure, the mass-averaged enthalpy at the mixing pressure, and the mass-averaged composition of the streams being mixed.

The two mixtures most pertinent to cycle calculations are those representing the composite exhaust gas, at exhaust conditions, issuing from the cylinder through the exhaust valve and the fresh charge, at manifold conditions, entering the cylinder through the intake valve. The state of the composite exhaust gas, corresponding to an average over the cycle, is designated by the values of p_e, $h^{(e)}$, and $n_\lambda^{(e)}$, where the composition and enthalpy values are the values of $\bar{\psi}^{(-)}(\theta_c^{(-)})$ for ψ equal to n_λ and the downstream enthalpy, respectively, for flow through the exhaust valve. The $n_\lambda^{(e)}$ and $h^{(e)}$ are calculated at $\theta_c^{(-)}$, the earliest point in the cycle when these numbers are available. The upstream state of the fresh charge to the cylinder is defined by the values of p_m, $h^{(0)}$, and $n_\lambda^{(0)}$. The composition and enthalpy values are affected not only by the reactant properties at the manifold conditions, but also by the cycle-averaged exhaust gas properties at the manifold conditions if there is any exhaust gas recirculation. Thus $n_\lambda^{(0)}$ and $h^{(0)}$ cannot be calculated until the exhaust valve closes. Since at this crankangle the intake valve may already be open (because of valve overlap) the properties of the fresh charge are not recalculated until the intake valve closes at $\theta_c^{(+)}$.

Flow stream properties: The foregoing discussions of flow and mixing permit a straightforward and relatively simple definition of the flow-related functions $\tilde{n}_\lambda^{(\pm)}$, $\tilde{h}^{(\pm)}$, $\tilde{n}_\lambda^{(1,-)}$, and $\tilde{h}_1^{(-)}$, which still remain undefined in equations (I-72) and (I-74). As a general guide to their prescription I shall assume that any material that flows out through the intake system must completely return to the cylinder before fresh charge is permitted to flow into the system. Similarly, in any given cycle, if a flow reversal occurs in the exhaust, then the material which left the cylinder during the current cycle will be returned to the cylinder. If all of the exhaust from the current cycle has been returned and the flow is still reversed, then the composite exhaust from the previous cycle will be used. For the composition-related functions we have

$$\tilde{n}_\lambda^{(+)} = \begin{cases} n_\lambda & \dot{M}^{(+)} < 0 \\ \bar{n}_\lambda^{(+)} & \dot{M}^{(+)} > 0,\ M^{(+)} < 0 \\ n_\lambda^{(0)} & \dot{M}^{(+)} > 0,\ M^{(+)} \geq 0 \end{cases}$$

$$\tilde{n}_\lambda^{(-)} = \begin{cases} n_\lambda & \dot{M}^{(-)} < 0 \\ \bar{n}_\lambda^{(-)} & \dot{M}^{(-)} > 0,\ M^{(-)} < 0 \\ n_\lambda^{(e)} & \dot{M}^{(-)} > 0,\ M^{(-)} \geq 0 \end{cases} \tag{I-121}$$

$$\tilde{n}_\lambda^{(1,-)} = \begin{cases} n_\lambda^{(1)} & \dot{M}^{(-)} < 0 \\ \bar{n}_\lambda^{(-)} & \dot{M}^{(-)} > 0,\ M^{(-)} < 0 \\ n_\lambda^{(e)} & \dot{M}^{(-)} > 0,\ M^{(-)} \geq 0 \end{cases}$$

which are consistent with the description just given. These functions are piecewise constant except when $\dot{M}^{(\pm)} < 0$, when they are clearly functions of crankangle. The enthalpy-related functions are similar, but for $\dot{M}^{(\pm)} > 0$ we must take into account that the state changes during flow. Thus we write

$$\tilde{h}^{(+)} = \begin{cases} h & \dot{M}^{(+)} < 0 \\ ('\bar{h}^{(+)})' & \dot{M}^{(+)} > 0,\ M^{(+)} < 0 \\ (h^{(0)})' & \dot{M}^{(+)} > 0,\ M^{(+)} \geq 0 \end{cases}$$

$$\tilde{h}^{(-)} = \begin{cases} h & \dot{M}^{(-)} < 0 \\ ('\bar{h}^{(-)})' & \dot{M}^{(-)} > 0,\ M^{(-)} < 0 \\ (h^{(e)})' & \dot{M}^{(-)} > 0,\ M^{(-)} \geq 0 \end{cases} \tag{I-122}$$

$$\tilde{h}_1^{(-)} = \begin{cases} h_1 & \dot{M}^{(-)} < 0 \\ ('\bar{h}^{(-)})' & \dot{M}^{(-)} > 0,\ M^{(-)} < 0 \\ (h^{(e)})' & \dot{M}^{(-)} > 0,\ M^{(-)} \geq 0 \end{cases}$$

where $'\bar{h}^{(\pm)}$ represents the average of the downstream enthalpy during efflux, and the notation $(\ )'$ refers to the downstream value during influx.

Ignition and flame front behavior: There are still two related items which need discussion before we have a completely defined model for the internal combustion engine. One is the flame ignition process and the effect of flame passage on the burned gas; the other is the definition of the functions which multiply $\dot{M}_b$ on the right side of equations in (I–74). Since I have already said that the combustion phase of the cycle begins with 0.01 mass percent of the unburned gas converted to burned gas, it must be the ignition process which is responsible for this conversion. It generates initial values for the combustion phase of the cycle. The ignition process is defined to be the conversion of 0.01 mass percent of unburned gas to the thermodynamic equilibrium state corresponding to the pressure and enthalpy of the unburned gas at the point of ignition. During the combustion phase the passage of the flame front through the unburned gas will be assumed to produce one of two possible effects. First, it may convert the freshly engulfed mass into the thermodynamic equilibrium state corresponding to the pressure and enthalpy of the unburned gas at that point and then mix it with the burned gas. This may be viewed as a variant of the global combustion model which has become popular in the treatment of combustion problems for which detailed reaction mechanisms and rates are unknown. In this case the rate is determined by $\dot{M}_b$, and the reaction products are specified by the equilibrium condition. When detailed reaction mechanism and rates are known for the reactants, one can dispense with the equilibrium condition. In this situation the passage of the flame front merely serves to incorporate some of the unburned gas with the burned gas, where its subsequent reaction is governed by chemical kinetics. The functions $\tilde{h}_1^{(b)}$, $\tilde{h}_2^{(b)}$, $n_\lambda^{(1,b)}$, and $n_\lambda^{(2,b)}$ are chosen to be consistent with this discussion

$$\tilde{h}_1^{(b)} = h_2 = \tilde{h}_2^{(b)}, \quad \tilde{n}_\lambda^{(2,b)} = n_\lambda^{(2)}$$

$$\tilde{n}_\lambda^{(1,b)} = \begin{cases} n_\lambda^{(\mathrm{eq})} & \text{(global combustion mechanism)} \\ \\ n_\lambda^{(2)} & \text{(detailed combustion mechanism)} \end{cases} \tag{I-123}$$

In equations (I-123) $n_\lambda^{(\mathrm{eq})}$ is the equilibrium composition of the flame zone calculated for the conditions existing in the unburned gas at the moment it is engulfed by the flame front. The choice for $\tilde{n}_\lambda^{(2,b)}$, in conjunction with earlier choices made for some of the other modeling functions, reduces the equation for $n_\lambda^{(2)}$ to $dn_\lambda^{(2)}/d\theta = 0$.

First specialization – simplified intake and exhaust. – The first specialization of the general model is largely a simplification of the treatment of flows through the intake and exhaust systems. This is augmented with the requirement that all chemical reactions cease in the burned gas at $\theta = 3\pi$ (of course, modulo 4π). Chemical reactions do not recommence until the inception of combustion on the following cycle. If the combustion phase extends to $\theta = 3\pi$, then at that point all reaction ceases and the burned and unburned gases are mixed at constant pressure and enthalpy.

Flows in the intake system are permitted only in the crankangle interval $0 \leq \theta \leq \pi$, while exhaust flows are confined to the interval $3\pi \leq \theta \leq 4\pi$; there is no valve overlap. The flows also take place without a pressure drop across the valves. The exhaust valve opens at $\theta_o^{(-)} = 3\pi$ (modulo 4π) and closes at $\theta_c^{(-)} = 4\pi$ (modulo 4π). If $p(3\pi) \neq p_e$, then there is an instantaneous change of state by one of the thermodynamic processes (I-118) to convert the pressure to p_e. If $p(3\pi) > p_e$, then the pressure is reduced to p_e and this is accompanied by a sudden reduction in mass (blowdown). If $p(3\pi) < p_e$, then the pressure is increased to p_e and this is accompanied by a sudden addition of composite exhaust gas from the previous cycle. When $p(3\pi)$ has been adjusted so that $p(3\pi) = p_e$, any additional flow through the exhaust system is determined by the condition $p = p_e$. Any reverse flow, if it occurs at all, will alter only the mass of the working fluid but not its temperature or composition. The intake valve opens no sooner then $\theta_o^{(+)} = 0$ (modulo 4π). If $p(0) < p_m$, then the valve opens at $\theta_o^{(+)} = 0$ and the pressure is instantaneously adjusted to p_m, by one of the processes (I-118), and accompanied by the addition of fresh charge (supercharging). If $p(0) \geq p_m$, then intake valve opening is delayed to the crankangle for which $p(\theta_o^{(+)}) = p_m$. Additional flow is such as to maintain $p = p_m$. The intake valve closes at $\theta_c^{(+)} = \pi$(modulo 4π). This prescription entirely avoids reverse flows in the intake system.

These assumptions produce a considerable simplification in equations (I–72) for the noncombustion phase of the cycle. The form of the equations changes with crankangle interval. The first member of equation (I–72) applies to all crankangle intervals, and it is supplemented by the following equations:

$0 \le \theta \le \theta_o^{(+)}$ and $\pi = \theta_c^{(+)} \le \theta \le \theta_0$:

$$\frac{du}{d\theta} = -\frac{p}{\rho}\frac{d \ln V}{d\theta} - \frac{\dot{Q}}{M\omega}, \quad \frac{dn_\lambda}{d\theta} = 0, \quad \frac{dM}{d\theta} = 0$$

$\theta_o^{(+)} \le \theta \le \theta_c^{(+)} = \pi$:

$$\frac{dh}{d\theta} = -\frac{\dot{Q}}{M\omega} + \left[h^{(0)} - h\right]\frac{d \ln M}{d\theta}, \quad \frac{dn_\lambda}{d\theta} = \left[n_\lambda^{(0)} - n_\lambda\right]\frac{d \ln M}{d\theta}, \quad \frac{dp}{d\theta} = 0$$

$\theta^* \le \theta \le \theta_o^{(-)} = 3\pi$: (I–124)

$$\frac{du}{d\theta} = -\frac{p}{\rho}\frac{d \ln V}{d\theta} - \frac{\dot{Q}}{M\omega}, \quad \frac{dn_\lambda}{d\theta} = \frac{R_\lambda}{\rho\omega}, \quad \frac{dM}{d\theta} = 0$$

$3\pi = \theta_o^{(-)} \le \theta \le \theta_c^{(-)} = 4\pi$

$$\frac{dh}{d\theta} = -\frac{\dot{Q}}{M\omega}, \quad \frac{dn_\lambda}{d\theta} = 0, \quad \frac{dp}{d\theta} = 0$$

There is also a simplification in the equations for the combustion phase (eqs. (I–74)).

$\theta_0 \le \theta \le \theta^*$:

$$\frac{d \ln \rho_1}{d\theta} = \frac{d \ln M_1}{d\theta} - \frac{d \ln V_1}{d\theta}, \quad \frac{du_1}{d\theta} = -\frac{p_1}{\rho_1}\frac{d \ln V_1}{d\theta} - \frac{\dot{Q}_1}{M_1\omega} + (h_2 - u_1)\frac{d \ln M_1}{d\theta}$$

$$\frac{dn_\lambda^{(1)}}{d\theta} = \frac{R_\lambda^{(1)}}{\rho_1\omega} + \left[\tilde{n}_\lambda^{(1,b)} - n_\lambda^{(1)}\right]\frac{d \ln M_1}{d\theta}, \quad \frac{d \ln \rho_2}{d\theta} = \frac{d \ln M_2}{d\theta} - \frac{d \ln V_2}{d\theta} \qquad \text{(I–125)}$$

$$\frac{du_2}{d\theta} = -\frac{p_2}{\rho_2}\frac{d \ln V_2}{d\theta} - \frac{\dot{Q}_2}{M_2\omega} + (h_2 - u_2)\frac{d \ln M_2}{d\theta}, \quad \frac{dn_\lambda^{(2)}}{d\theta} = 0$$

While fresh charge is being admitted to the cylinder, $\theta_o^{(+)} \le \theta \le \theta_c^{(+)}$, the function $n_\lambda^{(0)}$ is constant and both the composition and pressure equations can be integrated immediately. Only one equation, for the enthalpy, requires numerical integration. The integral of the composition equations has a simple form.

$$n_\lambda(\theta) = \frac{\left[n_\lambda\left(\theta_o^{(+)}\right) + E_m n_\lambda^{(0)}\right]}{1 + E_m}$$

(I–126)

$$E_m(\theta) \equiv \frac{\left[M(\theta) - M\left(\theta_o^{(+)}\right)\right]}{M\left(\theta_o^{(+)}\right)}$$

A similar situation exists during exhaust, $\theta_o^{(-)} \leq \theta \leq \theta_c^{(-)}$, where again only the enthalpy equation must be solved numerically. During the exhaust portion of the cycle it is convenient to work directly with the enthalpy equation. However, during the charging process it is more convenient to integrate an equation for the density. The correct evolution equation for the density is easily obtained from thermodynamic considerations. Thermodynamically we may write

$$\begin{aligned} &h = h(T, p, n_\lambda) \\ &p = p(T, \rho, n_\lambda) \end{aligned} \qquad \text{(I-127)}$$

and by differentiation, using the differential equations for the interval $\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)}$, we obtain a pair of equations for $d \ln T/d\theta$ and $d \ln M/d\theta$.

$$\frac{d \ln T}{d\theta} + \left(\frac{\partial h}{\partial \ln T}\right)^{-1} \left[h - h^{(0)} + \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial h}{\partial n_\lambda}\right] \frac{d \ln M}{d\theta} = -\frac{\dot{Q}}{M\omega} \left(\frac{\partial h}{\partial \ln T}\right)^{-1}$$

$$\frac{\partial \ln p}{\partial \ln T} \frac{d \ln T}{d\theta} + \left[\frac{\partial \ln p}{\partial \ln \rho} + \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial \ln p}{\partial n_\lambda}\right] \frac{d \ln M}{d\theta} = \frac{\partial \ln p}{\partial \ln \rho} \frac{d \ln V}{d\theta}$$

Solving for $d \ln M/d\theta$ gives

$$\frac{d \ln M}{d\theta} = \frac{\dfrac{\partial \ln p}{\partial \ln \rho} \dfrac{d \ln V}{d\theta} + \dfrac{\partial \ln p}{\partial \ln T} \dfrac{\dot{Q}}{M\omega(\partial h/\partial \ln T)}}{\dfrac{\partial \ln p}{\partial \ln \rho} + \left(n_\lambda^{(0)} - n_\lambda\right) \dfrac{\partial \ln p}{\partial n_\lambda} - \dfrac{\partial \ln p}{\partial \ln T} \left(\dfrac{\partial h}{\partial \ln T}\right)^{-1} \left[h - h^{(0)} + \left(n_\lambda^{(0)} - n_\lambda\right) \dfrac{\partial h}{\partial n_\lambda}\right]}$$

If we substitute this into the first member of equations (I-72), we obtain an equation for the density.

$$\begin{aligned} \frac{d \ln \rho}{d\theta} = &\left(\frac{\partial \ln p}{\partial \ln T} \frac{\dot{Q}}{M\omega(\partial h/\partial \ln T)} + \left\{\frac{\partial \ln p}{\partial \ln T} \left(\frac{\partial h}{\partial \ln T}\right)^{-1} \right.\right. \\ &\left.\left. \times \left[h - h^{(0)} + \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial h}{\partial n_\lambda}\right] - \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial \ln p}{\partial n_\lambda}\right\} \frac{d \ln V}{d\theta}\right) \Bigg/ \\ &\left\{\frac{\partial \ln p}{\partial \ln \rho} + \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial \ln p}{\partial n_\lambda} - \frac{\partial \ln p}{\partial \ln T} \left(\frac{\partial h}{\partial \ln T}\right)^{-1} \left[h - h^{(0)} + \left(n_\lambda^{(0)} - n_\lambda\right) \frac{\partial h}{\partial n_\lambda}\right]\right\} \end{aligned}$$

Both the differential equation for mass and the differential equation for density can be simplified if one realizes that h is homogeneous of degree one in n_λ for then $n_\lambda\ \partial h/\partial n_\lambda = h$.

$$\frac{d \ln M}{d\theta} = \frac{\dfrac{\partial \ln p}{\partial \ln \rho} \dfrac{d \ln V}{d\theta} + \dfrac{\partial \ln p}{\partial \ln T} \dfrac{\dot{Q}}{M\omega(\partial h/\partial \ln T)}}{\dfrac{\partial \ln p}{\partial \ln \rho} + \left[n_\lambda^{(0)} - n_\lambda\right] \dfrac{\partial \ln p}{\partial n_\lambda} - \dfrac{\partial \ln p}{\partial \ln T}\left(\dfrac{\partial h}{\partial \ln T}\right)^{-1}\left[n_\lambda^{(0)} \dfrac{\partial h}{\partial n_\lambda} - h^{(0)}\right]} \qquad \left(\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)}\right)$$

(I–128a)

$$\frac{d \ln \rho}{d\theta} = \frac{\dfrac{\partial \ln p}{\partial \ln T} \dfrac{\dot{Q}}{M\omega c_p T} + \left\{\dfrac{\partial \ln p}{\partial \ln T}\left(\dfrac{\partial h}{\partial \ln T}\right)^{-1}\left[n_\lambda^{(0)} \dfrac{\partial h}{\partial n_\lambda} - h^{(0)}\right] - \left(n_\lambda^{(0)} - n_\lambda\right) \dfrac{\partial \ln p}{\partial n_\lambda}\right\} \dfrac{d \ln V}{d\theta}}{\dfrac{\partial \ln p}{\partial \ln \rho} + \left(n_\lambda^{(0)} - n_\lambda\right) \dfrac{\partial \ln p}{\partial n_\lambda} - \dfrac{\partial \ln p}{\partial \ln T}\left(\dfrac{\partial h}{\partial \ln T}\right)^{-1}\left[n_\lambda^{(0)} \dfrac{\partial h}{\partial n_\lambda} - h^{(0)}\right]}$$

$$\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)}$$

The density equation becomes the replacement equation for the enthalpy evolution equation for $\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)}$. The corresponding equations for the interval $\theta_o^{(-)} \leq \theta \leq \theta_c^{(-)}$ can be obtained from equation (I–128a) by letting $n_\lambda^{(0)} = n_\lambda$ and $h^{(0)} = h$, but, of the two, only the expression for $d \ln M/d\theta$ will be used there.

The numerator in the expression for $d \ln M/d\theta$ in equation (I–128a) could, in rare circumstances, be negative for intake flows near $\theta = \pi$, and this is inconsistent with the assumption of no reverse flows in the intake system. The inconsistency can be removed when $\dot{Q} \leq 0$ by setting $d \ln M/d\theta = 0$. This, in effect, redefines the heat loss as

$$\frac{\dot{Q}}{M\omega c_p T} \equiv - \frac{\partial \ln p}{\partial \ln \rho} \frac{d \ln V}{d\theta} \bigg/ \left(\frac{\partial \ln p}{\partial \ln T}\right) \leq 0 \qquad \text{(I–128b)}$$

if $T \leq T_w$. Such a procedure is not possible when $T > T_w$ since this implies that $\dot{Q} > 0$.

Second specialization – equilibrium chemistry. – The second specialization superimposes on the equations of the preceding section a simplification of the treatment of the chemistry. In the first level of specialization, chemical kinetics was applied to the burned gases in the combustion and postcombustion portions of the cycle $\left(\theta_0 \leq \theta \leq \theta_o^{(-)}\right)$. At this level we now replace chemical kinetics with equilibrium chemistry by disregarding the differential equations for the composition variables. During combustion $(\theta_0 \leq \theta \leq \theta^*)$ they are replaced by the assumption that the burned gas is in chemical equilibrium. In the postcombustion portion of the cycle $\left(\theta^* \leq \theta \leq \theta_o^{(-)}\right)$, all chemical species in the burned gas are assumed to be in chemical equilibrium except for the oxide of nitrogen (NO), which is assumed to be nonreacting.

Third specialization – instantaneous combustion and no heat transfer. – At this, the lowest level of modeling, the combustion interval is shrunk to zero, and the combustion process is modeled as the instantaneous conversion of the unburned gas to burned gas at the moment of ignition. The composition of the burned gas is that corresponding to the thermodynamic equilibrium state at fixed volume and internal energy. Throughout the cycle no heat is transferred to or from the working fluid. These assumptions effect a drastic simplification in those equations in (I–124) which still govern the model cycle. It is no longer necessary to solve systems of differential equations numerically, for all of them can now be integrated analytically and the cycle calculation is reduced to solving ordinary systems of equations.

During the intake portion of the cycle $(\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)} = \pi)$, the sole remaining equation is the one for the enthalpy. But in the absence of heat transfer it takes the form

$$\frac{dh}{d\theta} = \left[h^{(0)} - h\right] \frac{d \ln M}{d\theta}$$

whose integration gives a result identical in structure to equation (I–126).

$$h(\theta) = \frac{h\left(\theta_0^{(+)}\right) + E_m h^{(0)}}{1 + E_m} \tag{I–129}$$

During the exhaust portion of the cycle $(3\pi = \theta_o^{(-)} \leq \theta \leq \theta_c^{(-)} = 4\pi)$ the enthalpy remains constant. Consequently the state of the working fluid is constant during the exhaust. The only differential equation which remains to be considered is for the internal energy which occurs in three segments of the cycle. But under the assumed conditions we have

$$\frac{du}{d\theta} = -\frac{p}{\rho} \frac{d \ln V}{d\theta} = \frac{p}{\rho} \frac{d \ln \rho}{d\theta}$$

and comparing it to the first law of thermodynamics (eq. (I–79)) we see that this implies $ds/d\theta = 0$. Thus the crankangle intervals $0 \leq \theta \leq \theta_o^{(+)}$, $\pi = \theta_c^{(+)} \leq \theta \leq \theta_0$ and $\theta^* \leq \theta \leq \theta_o^{(-)} = 3\pi$ are thermodynamically isentropic processes with fixed composition except at the point of combustion.

The only portion of the cycle still undefined is the treatment of the potential discontinuities at $\theta_o^{(+)} = 0$ (if $p(0) < p_m$) and $\theta_o^{(-)} = 3\pi$ (if $p(3\pi) \neq p_e$). The definition is completed by requiring the working fluid to undergo one of the changes of state given in equation (I–118).

The net result of all of the simplifications is that this model of the internal combustion engine becomes a completely thermodynamic one. No vestiges of the rate processes remain in the calculation of this, the most highly idealized model. Its evaluation does not require the numerical integration of even a single differential equation.

Physical Properties

The governing equations and the physical properties used in the solution of those equations represent two independent components of every model of a physical system. The results of the computation are influenced as much by one as by the other. It makes little sense to construct an elaborate model and then to compromise the results obtained from the model with grossly inadequate physical properties. Naturally there will be occasions when only poor estimates of physical properties are available. Under such circumstances one is forced to use the poor data. But when better data are easily obtained from the literature, it seems to me that it is a false economy to ignore it and then pay the price of an uncertainty in results.

There are three categories of physical property data which are needed in the model of the internal combustion engine. They are the thermodynamic, the chemical kinetic, and the transport properties. Each will be discussed separately.

Thermodynamic properties. – In the internal combustion engine under typical operating conditions one can expect to encounter temperatures that range from near room temperature to almost 3000 K. Similarly pressures could vary from subatmospheric to, perhaps, something of the order of 15 atmospheres. Experience has shown that over this range of conditions the actual thermodynamic properties of a gaseous mixture will differ inconsequentially from properties based on the independent species approximation. This approximation calculates mixture properties as a superposition of pure-species properties, which themselves may vary with temperature but not with pressure and composition. The Gibbs free energy per unit mass g has a very simple appearance

$$g=\sum_{\lambda} n_{\lambda}\left[{}^{*}\mu^{\lambda}(T)+RT\ln\left(\frac{p n_{\lambda}}{\sum_{\nu} n_{\nu}}\right)\right] \tag{I-130}$$

where summations have been written explicitly. The temperature-dependent function ${}^{*}\mu^{\lambda}(T)$ is the 1-atmosphere approximation to the pure-species chemical potential. Expressions for the enthalpy and the entropy are obtained from the Gibbs free energy by differentiation

$$\begin{aligned} h &\equiv -T^{2}\frac{\partial(g/T)}{\partial T}=-T^{2}\sum_{\lambda} n_{\lambda}\frac{\partial({}^{*}\mu^{\lambda}/T)}{\partial T}={}^{*}H^{\lambda}n_{\lambda} \\ s &= -\frac{\partial g}{\partial T}=\sum_{\lambda} n_{\lambda}\left[-\frac{\partial^{*}\mu^{\lambda}}{\partial T}-R\ln\left(\frac{p n_{\lambda}}{\sum_{\nu} n_{\nu}}\right)\right]=\sum_{\lambda} n_{\lambda}\left[{}^{*}S^{\lambda}-R\ln\left(\frac{p n_{\lambda}}{\sum_{\nu} n_{\nu}}\right)\right] \end{aligned} \tag{I-131}$$

where the summation convention has been reintroduced in the last expression for the enthalpy. The equation of state also follows by differentiation of the Gibbs free energy

$$\rho^{-1}=\frac{\partial g}{\partial p}=\frac{\left(RT\sum_{\lambda} n_{\lambda}\right)}{p} \tag{I-132}$$

which is obviously the ideal-gas equation of state. The internal energy takes on a simple form which is obtained from the expression for h and the equation of state.

$$\begin{aligned} u &= h-\frac{p}{\rho}={}^{*}U^{\lambda}n_{\lambda} \\ {}^{*}U^{\lambda}(T) &\equiv {}^{*}H^{\lambda}(T)-RT \end{aligned} \tag{I-133}$$

The partial molar properties are also quite simple.

$$\begin{aligned} &\mu^{\lambda}\equiv\frac{\partial g}{\partial n_{\lambda}}={}^{*}\mu^{\lambda}+RT\ln\left(\frac{p n_{\lambda}}{\sum_{\nu} n_{\nu}}\right),\quad H^{\lambda}\equiv\frac{\partial h}{\partial n_{\lambda}}={}^{*}H^{\lambda}(T) \\ &S^{\lambda}\equiv\frac{\partial s}{\partial n_{\lambda}}={}^{*}S^{\lambda}-RT\ln\left(\frac{p n_{\lambda}}{\sum_{\nu} n_{\nu}}\right) \\ &V^{\lambda}\equiv\frac{\partial(\rho^{-1})}{\partial n_{\lambda}}=\frac{RT}{p},\quad U^{\lambda}\equiv\frac{\partial u}{\partial n_{\lambda}}={}^{*}U^{\lambda}(T) \end{aligned} \tag{I-134}$$

There are some additional derivatives which are needed. For example, with equation (I-128) we need

$$\begin{aligned} &\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_{\lambda}}=1=\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_{\lambda}} \\ &\left(\frac{\partial\ln p}{\partial n_{\lambda}}\right)_{T,\rho}=\left(\sum_{\tau} n_{\tau}\right)^{-1} \end{aligned} \tag{I-135}$$

which are obtained by direct differentiation of the equation of state (I–132). The evaluation of the thermodynamic derivatives which appear in equation (I–78) is a bit more complex for it requires not only the differentiation of the equation of state but also an application of the chain rule for differentiation.

$$\left(\frac{\partial \ln p}{\partial u}\right)_{\rho,n_\lambda} = \left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda} \left(\frac{\partial \ln T}{\partial u}\right)_{\rho,n_\lambda}$$

$$\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{u,n_\lambda} = \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{T,n_\lambda} + \left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda} \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_{u,n_\lambda}$$

$$\left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{u,\rho} = \left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda} \left(\frac{\partial \ln T}{\partial n_\lambda}\right)_{u,\rho} + \left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{T,\rho}$$

The pressure derivatives which appear in these formulas can be taken from equations (I–135), while $(\partial \ln T/\partial u)_{\rho,n_\lambda} = \left[T(\partial u/\partial T)_{\rho,n_\lambda}\right]^{-1}$ can be calculated by direct differentiation of the expression for u (eq. (I–133)). The two remaining temperature derivatives must still be put into a form that is suitable for direct evaluation. The temperature derivative with respect to density may be expressed as

$$\left(\frac{\partial \ln T}{\partial \ln \rho}\right)_{u,n_\lambda} = -\frac{(\partial u/\partial \ln \rho)_{T,n_\lambda}}{(\partial u/\partial \ln T)_{\rho,n_\lambda}}$$

But from equation (I–133) it follows that the density derivative of the internal energy vanishes, and so

$$\left(\frac{\partial \ln T}{\partial \ln \rho}\right)_{u,n_\lambda} = 0 = \left(\frac{\partial u}{\partial \ln \rho}\right)_{T,n_\lambda}$$

follows immediately. Similarly

$$\left(\frac{\partial \ln T}{\partial n_\lambda}\right)_{u,\rho} = -\frac{(\partial u/\partial n_\lambda)_{T,\rho}}{(\partial u/\partial \ln T)_{n_\lambda,\rho}}$$

and the two derivatives on the right side can be evaluated by differentiation of the expression for the internal energy (eq. (I–133)). The final results are

$$\left(\frac{\partial \ln p}{\partial u}\right)_{\rho,n_\lambda} = \left[n_\lambda \frac{\partial^* U^\lambda}{\partial \ln T}\right]^{-1} = \left[T n_\lambda {}^*C^\lambda\right]^{-1}, \quad \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{u,n_\lambda} = 1$$

$$\left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{u,\rho} = \left(\sum_\tau n_\tau\right)^{-1} - {}^*U^\lambda \left[n_\tau \frac{\partial^* U^\tau}{\partial \ln T}\right]^{-1} \tag{I–136}$$

$$= \left(\sum_\tau n_\tau\right)^{-1} - {}^*U^\lambda \left[T n_\tau {}^*C^\tau\right]^{-1} = \left(\sum_\tau n_\tau\right)^{-1} - {}^*U^\lambda \left(\frac{\partial \ln p}{\partial u}\right)_{\rho,n_\lambda}$$

and are to be used in equation (I–78). There are some additional thermodynamic derivatives which will be used during cycle calculations. These fall into two categories: conventional partial derivatives and partial derivatives when the composition is in chemical equilibrium. The first category is quite simple.

$$\left(\frac{\partial h}{\partial T}\right)_{p,n_\lambda} {}^{*}C^{\lambda}n_\lambda + R\sum_{\lambda} n_\lambda = \frac{1}{(\partial T/\partial h)_{p,n_\lambda}},\ \left(\frac{\partial h}{\partial p}\right)_{T,n_\lambda} = 0,\ \left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T} = {}^{*}H_\lambda, \tag{I-137a}$$

$$\left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda} = \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{T,n_\lambda} = \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_{T,n_\lambda} = -\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_{p,n_\lambda} = 1,\ \left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{T,\rho} = \left(\sum_{\tau} n_\tau\right)^{-1}$$

The second category of derivatives contains contributions from reactions and so is more complex.

$$\left(\frac{\partial h}{\partial T}\right)_p \equiv c_p,\ \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T = 1 - \left(\frac{\partial \ln \sum_{\tau} n_\tau}{\partial \ln p}\right)_T$$

$$\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p = -\left[1 + \left(\frac{\partial \ln \sum_{\tau} n_\tau}{\partial \ln T}\right)_p\right]$$

$$\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_u = \left[p^{-1}\rho T c_p + \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p\right] \Big/ \left[p^{-1}\rho T c_p \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p^2\right] \tag{I-137b}$$

$$\left(\frac{\partial \ln p}{\partial u}\right)_\rho = -p^{-1}\rho\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \Big/ \left[p^{-1}\rho T c_p \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p^2\right]$$

$$\left(\frac{\partial \ln T}{\partial \ln \rho}\right)_u = -\left[\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p + \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T\right] \Big/ \left[p^{-1}\rho T c_p \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p^2\right]$$

$$\left(\frac{\partial \ln T}{\partial u}\right)_\rho \equiv \left(T c_v\right)^{-1} = p^{-1}\rho T c_p \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T \Big/ T c_p \left[p^{-1}\rho T c_p \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_T - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p^2\right]$$

The numerical intricacies of thermodynamic calculations at this level of approximation are well understood and have been reviewed by Zeleznik and Gordon (ref. 52). Furthermore a much tested and broadly disseminated third-generation computer program, written by Gordon and McBride (ref. 53), is available for performing the thermodynamic calculations, and there exists a large compendium of data (ref. 54) which can be used with it. All thermodynamic calculations for the model of the internal combustion engine will be based on this computer program.

Chemical kinetic properties. – Chemical kinetics makes its contribution to modeling by providing expressions for the net volumetric species production rates R_λ and by supplying experimental estimates of the values for parameters in these expressions. All chemical changes are ascribed to elementary, or simple, reactions which combine to generate an overall mechanism for the change. The rates of these elementary processes are assumed to be proportional to the volumetric concentration of each reactant raised to some power and are dependent on temperature. A copious literature exists on the rates of elementary reactions, including some extensive compilations and critical evaluations (refs. 55 and 56).

Each elementary reaction, called a forward reaction, in a reaction mechanism is presumed to be accompanied by another reaction, called the backward or reverse reaction, which is its exact inverse. Generally, but not universally, the ratio of the forward reaction rate constant to the backward reaction rate constant is assumed to be equal to the equilibrium constant for the related "thermodynamic reaction." Some elementary reactions involve species which participate in the reaction but which are not chemically affected themselves. Such inert species are sometimes spoken of as "third bodies" and such reactions are known as "third-body reactions." The inert species in third-body reactions can be any species present in the reacting mixture.

I now seek to generate a concise expression for R_λ from a postulated reaction mechanism. To this end let me assume that each forward-backward pair of elementary reactions in a mechanism is labeled by a pair of indices, one Latin and one Greek. The Latin index, say j, will have the range $j=1, 2, \ldots, N_R$ and labels the distinct elementary reaction pairs. Two elementary reaction pairs which differ only in the choice of third body will not be considered to be distinguishable, and so j will label only one representative of given type of a third-body elementary reaction pair. The Greek index, from the last part of the alphabet, will be used to distinguish among the various third-body reactions of a given type by labeling them with the particular third body. Thus the Greek index will have a range determined by the type of reaction. The range will always be $1, 2, \ldots, N_j$, where $N_j=1$ if the jth distinct reaction pair is not a third-body reaction and $N_j=N$, where N equals the number of reacting species, for reactions which are of third-body type. This should cause no confusion for the N_j will appear explicitly in all formulas and any summation over the Greek index will in fact always correspond to the usual one, namely, over all species. This notational convention permits me to write the complete reaction mechanism quite concisely.

$$S^\lambda \nu_{\lambda j\sigma} \xrightleftharpoons[k_b(j\sigma)]{k_f(j\sigma)} S^\lambda \nu'_{\lambda j\sigma} \qquad \begin{matrix} j=1, 2, \ldots, N_R \\ \sigma=1, 2, \ldots, N_j \end{matrix} \tag{I-138}$$

Here S^λ are symbols for the chemical species, $\nu_{\lambda j\sigma}$ and $\nu'_{\lambda j\sigma}$ are the stoichiometric coefficients, and $k_f(j\sigma)$ and $k_b(j\sigma)$ are the forward and backward reaction rate constants. Consistent with my labeling of reaction pairs is the assumption that the stoichiometric coefficients have the form

$$\begin{aligned} \nu_{\lambda j\sigma} &= \nu_{\lambda j} + \delta_{N,N_j}\delta_{\lambda\sigma} \\ \nu'_{\lambda j\sigma} &= \nu'_{\lambda j} + \delta_{N,N_j}\delta_{\lambda\sigma} \end{aligned} \tag{I-139}$$

and that the forward and backward rate constants satisfy the constraint

$$\frac{k_f(j\sigma)}{k_b(j\sigma)} \equiv K_j = \prod_\lambda \left(\rho n_\lambda^{(\mathrm{eq})}\right)^{\nu'_{\lambda j}-\nu_{\lambda j}} \tag{I-140}$$

The right side of equation (I-140) should be recognized as the so-called equilibrium constant, based on volumetric concentration units, associated with the reaction pair (I-138), which is being regarded as a "thermodynamic reaction." The forward rate constant will be assumed to have the form

$$k_f(j\sigma) = k_f(j)\left(m_j^\sigma\right)^{\delta_{N,N_j}} \tag{I-141}$$

where m_j^σ is called the third-body efficiency and could, in principle, be a function of temperature. In practice, experimental data are usually only adequate to treat third-body efficiencies as temperature independent. The volumetric production rate R_λ for the mechanism (I-138) is the expression

$$R_\lambda \equiv \sum_{j=1}^{N_R} \sum_{\sigma=1}^{N_j} \left(\nu'_{\lambda j\sigma} - \nu_{\lambda j\sigma}\right) \left[k_f(j\sigma)\prod_\tau (\rho n_\tau)^{\nu_{\tau j\sigma}} - k_b(j\sigma)\prod_\tau (\rho n_\tau)^{\nu'_{\tau j\sigma}}\right] \tag{I-142}$$

which can be simplified considerably. Clearly because of the structure of the stoichiometric coefficients (eq. (I–139)), we can write

$$\prod_{\tau} (\rho n_{\tau})^{\nu_{\tau j\sigma}} = (\rho n_{\sigma})^{\delta_{N,N_j}} \prod_{\tau} (\rho n_{\tau})^{\nu_{\tau j}}$$

and because of the structure of the forward rates (eq. (I–141)) we can write

$$\sum_{\sigma=1}^{N_j} k_f(j\sigma)(\rho n_{\sigma})^{\delta_{N,N_j}} = k_f(j)\left(\rho m_j^{\sigma} n_{\sigma}\right)^{\delta_{N,N_j}}$$

and these results can be used to simplify R_{λ}.

$$R_{\lambda} = \sum_{j=1}^{N_R} \left(\nu'_{\lambda j} - \nu_{\lambda j}\right) k_f(j) \left(\rho m_j^{\sigma} n_{\sigma}\right)^{\delta_{N,N_j}} \left[\prod_{\tau} (\rho n_{\tau})^{\nu_{\tau j}} - K_{\mathrm{j}}^{-1} \prod_{\tau} (\rho n_{\tau})^{\nu'_{\tau j}}\right] \tag{I–143}$$

An expression for K_j is easily obtained from the thermodynamic condition for equilibrium,

$$\left(\nu'_{\lambda j\sigma} - \nu_{\lambda j\sigma}\right)\mu^{\lambda} = \left(\nu'_{\lambda j} - \nu_{\lambda j}\right)\mu^{\lambda} = 0$$

combined with the expression for the chemical potential (I–134) and the equation of state (I–132). The result

$$K_j(T) = (RT)^{-\sum_{\lambda}\left(\nu'_{\lambda j} - \nu_{\lambda j}\right)} \exp\left[-\frac{\left(\nu'_{\tau j} - \nu_{\tau j}\right) {}^{*}\mu^{\tau}}{RT}\right] \tag{I–144}$$

is clearly a function of temperature alone. The temperature dependence of $k_f(j)$ is assumed to be of the form

$$k_f(j) = A_j T^{n_j} \exp[-E_j/RT] \tag{I–145}$$

where A_j is known as the preexponential factor and E_j is called the activation energy. Equations (I–143) to (I–145) define the volumetric production rate when coupled with the assumption that the third-body efficiencies are constants.

It will be necessary to have available the derivatives of R_{λ} with respect to temperature and composition. Since all of the temperature dependence of R_{λ} resides in K_j and $k_f(j)$, if third-body efficiencies are assumed to be temperature independent, we must calculate their derivatives. Using the thermodynamic relation $\partial(g/T)/\partial \ln T = -h/T$, we can easily show that

$$\frac{\partial \ln K_j}{\partial \ln T} = \frac{\left(\nu'_{\tau j} - \nu_{\tau j}\right) {}^{*}H^{\tau}}{RT} - \sum_{\lambda}\left(\nu'_{\lambda j} - \nu_{\lambda j}\right) \tag{I–146}$$

while the temperature derivative of $k_f(j)$ only requires direct differentiation.

$$\frac{\partial \ln k_f(j)}{\partial \ln T} = n_j + \frac{E_j}{RT} \tag{I–147}$$

The temperature derivative of R_{λ} can now be written in terms of the derivatives of K_j and $k_f(j)$.

$$\frac{\partial R_\lambda}{\partial \ln T} = \sum_{j=1}^{N_R} \left(\nu'_{\lambda j} - \nu_{\lambda j}\right) k_f(j) \left(\rho m_j^\sigma n_\sigma\right)^{\delta_{N,N_j}} \left[\prod_\tau (\rho n_\tau)^{\nu_{\tau j}} - K_j^{-1} \prod_\tau (\rho n_\tau)^{\nu'_{\tau j}}\right] \frac{\partial \ln k_f(j)}{\partial \ln T}$$

$$+ \sum_{j=1}^{N_R} \left(\nu'_{\lambda j} - \nu_{\lambda j}\right) k_f(j) \left(\rho m_j^\sigma n_\sigma\right)^{\delta_{N,N_j}} K_j^{-1} \prod_\tau (\rho n_\tau)^{\nu'_{\tau j}} \frac{\partial \ln K_j}{\partial \ln T} \tag{I-148}$$

The derivatives with respect to composition can be calculated by using the results

$$\frac{\partial \ln\left(\rho m_j^\sigma n_\sigma\right)^{\delta_{N,N_j}}}{\partial n_\lambda} = \delta_{N,N_j} \frac{\rho m_j^\lambda}{\left(\rho m_j^\sigma n_\sigma\right)^{\delta_{N,N_j}}} = \frac{\delta_{N,N_j}\, m_j^\lambda}{m_j^\sigma n_\sigma} \tag{I-149}$$

$$\frac{\partial}{\partial n_\lambda} \prod_\tau (\rho n_\tau)^{\nu_{\tau j}} = \begin{cases} \nu_{\lambda j} n_\lambda^{-1} \prod_\tau (\rho n_\tau)^{\nu_{\tau j}} & n_\lambda \neq 0 \\ \prod_{\tau \neq \lambda} (\rho n_\tau)^{\nu_{\tau j}} & n_\lambda = 0 \text{ and } \nu_{\lambda j} = 1 \\ 0 & n_\lambda = 0 \text{ and } \nu_{\lambda j} > 1 \end{cases} \tag{I-150}$$

for the derivatives of composition terms appearing in R_λ.

$$\frac{\partial R_\lambda}{\partial n_\sigma} = \sum_{j=1}^{N_R} \left(\nu'_{\lambda j} - \nu_{\lambda j}\right) k_f(j) \left(\rho m_j^\tau n_\tau\right)^{\delta_{N,N_j}} \left[\prod_\tau (\rho n_\tau)^{\nu_{\tau j}} - K_j^{-1} \prod_\tau (\rho n_\tau)^{\nu'_{\tau j}}\right] \frac{\partial \ln\left(\rho m_j^\tau n_\tau\right)^{\delta_{N,N_j}}}{\partial n_\sigma}$$

$$+ \sum_{j=1}^{N_R} \left(\nu'_{\lambda j} - \nu_{\lambda j}\right) k_f(j) \left(\rho m_j^\tau n_\tau\right)^{\delta_{N,N_j}} \left[\frac{\partial}{\partial n_\lambda} \prod_\tau (\rho n_\tau)^{\nu_{\tau j}} - K_j^{-1} \frac{\partial}{\partial n_\lambda} \prod_\tau (\rho n_\tau)^{\nu'_{\tau j}}\right] \tag{I-151}$$

The similarity in structure between R_λ and its derivatives means that the derivatives can be calculated with only a small expenditure of effort over what is required to calculate R_λ.

Transport properties. – The transport properties which are significant to the modeling of the internal combustion engine are the thermal conductivity k and the shear viscosity η of the working fluid. The viscosity is required for the calculation of Reynolds numbers, while the viscosity and the thermal conductivity are used to calculate the Prandtl number which appears in the expression for the heat transfer coefficient. Since the working fluid will usually be a complex mixture of many species, it is the mixture transport properties we want. Experimental data are, however, pretty much confined to pure species and binary mixtures. The resolution to the quandary lies in the use of mixture formulas which have been devised to express mixture transport properties in terms of the pure species properties η_λ and k_λ.

I have chosen to use the mixture formula proposed by Wilke (refs. 57 and 58) for the viscosity.

$$\eta = \sum_\lambda \eta_\lambda \left(\frac{n_\lambda}{\sum_\tau \phi_{\lambda\tau} n_\tau}\right)$$

$$\phi_{\lambda\tau} = \frac{\sqrt{2}\left[1 + \left(\frac{\eta_\lambda}{\eta_\tau}\right)^{1/2} \left(\frac{\mathcal{W}_\tau}{\mathcal{W}_\lambda}\right)^{1/4}\right]^2}{4\left[1 + \frac{\mathcal{W}_\lambda}{\mathcal{W}_\tau}\right]^{1/2}} \tag{I-152}$$

This viscosity formula is normally written in terms of mole fractions, but because it is homogeneous of degree zero in the composition variables, it can just as well be written in terms of the n_σ as was done here. The functions $\phi_{\lambda\tau}$, containing pure-species viscosities η_λ and molecular weights $\mathcal{W}_\lambda$, are not symmetric in the indices and reduce to unity for $\lambda = \tau$.

For the thermal conductivity I have elected to use a formula which is essentially that proposed by Lindsay and Bromley (ref. 59) and which has a structure quite similar to the viscosity formula. It can be written as

$$k = \sum_\lambda k_\lambda \left(\frac{n_\lambda}{\sum_\tau \phi_{\lambda\tau} n_\tau} \right)$$

$$\bar{\phi}_{\lambda\tau} = \frac{1}{4} \left\{ 1 + \left[\left(\frac{\eta_\lambda}{\eta_\tau} \right) \left(\frac{\mathcal{W}_\tau}{\mathcal{W}_\lambda} \right)^{3/4} \left(1 + \frac{C_\tau}{T} \right)^{-1} \left(1 + \frac{C_\lambda}{T} \right) \right]^{1/2} \right\}^2 \left(1 + \frac{C_{\lambda\tau}}{T} \right) \left(1 + \frac{C_\lambda}{T} \right)^{-1} \tag{I-153}$$

where k_λ is the pure-species thermal conductivity. The function $\bar{\phi}_{\lambda\tau}$ equals unity for $\lambda = \tau$. The C_λ and $C_{\lambda\tau}$ are known as Sutherland's constants, where $C_{\lambda\tau}$ is generally taken as proportional to the geometric mean of C_λ and C_τ. Lindsay and Bromley suggest taking the proportionality constant as unity except where one of the pair of species is highly polar, for which they suggest the use of 0.733. Because k is relatively insensitive to choices of C_λ, I have chosen to use unity for all pairs of species. The value of C_λ was approximated as 1½ times the normal boiling point by Lindsay and Bromley. It is, in fact, exactly defined by Sutherland's approximate formula for the temperature dependence of the pure-species viscosity (ref. 60)

$$\eta_\lambda \cong b_\lambda T^{1/2} \left(1 + \frac{C_\lambda}{T} \right)^{-1}$$

which is generally valid only for a very limited temperature interval when its two parameters are evaluated by fitting experimental data. But for the small range over which it is valid it implies that

$$1 + \frac{C_\lambda}{T} = \left[\frac{3}{2} - \frac{d \ln \eta_\lambda}{d \ln T} \right]^{-1} \tag{I-154}$$

and I shall use this as the defining equation for C_λ to be used with the thermal conductivity formula. The calculation of C_λ by equation (I-154) makes it a temperature-dependent function rather than a constant and of course so too is $C_{\lambda\tau}$.

$$C_{\lambda\tau} \equiv (C_\lambda C_\tau)^{1/2} \tag{I-155}$$

Appendix – Symbols

A	surface area
A_j	preexponential factor for forward rate constant, eq. (I-145)
$A^{(\pm)}$	poppet valve flow function, eq. (I-117a)
$A^{(\pm)}_{\text{flow}}$	cross-sectional flow area, eq. (I-116a)
$A^{(\pm)}_n$	$n=1, 2, 3$ poppet valve flow parameters, eq. (I-117a)
A/F	air to fuel weight (or mass) ratio
a	heat transfer coefficient parameter, eq. (I-105)
a_n	$n=1, 2, \ldots, 10$ parameters for Fourier burning law, eq. (I-92)
B	cylinder bore
b	heat transfer coefficient parameter, eq. (I-105)
b_1, b_2	parameters, eq. (I-108)
$b_{\alpha\beta}$	metric tensor for a two-dimensional subspace
$b^{(\pm)}$	poppet valve flow function, eq. (I-117a)
$b^{(\pm)}_n$	$n=1, 2, 3$ poppet valve flow parameters, eq. (I-117a)
C	closed curve on a surface
C_λ	Sutherland's constant, calculated by eq. (I-154)
$^*C^\lambda$	constant-volume heat capacity per mole of pure species λ
c_n	$n=1, 2, 3, 4$ heat transfer coefficient parameters, eq. (I-105)
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
$\mathrm{d}M^{\bar{\mu}}/\mathrm{d}t$	eq. (I-29)
$\mathrm{d}V^{\bar{\mu}}/\mathrm{d}t$	eq. (I-28)
$d^{(\pm)}$	minimum valve diameter for poppet valve
d^k_λ	molar diffusive flux vector for species λ
da	differential element of surface
dc	differential element of arc along curve C
dv	differential element of volume
E_G	mass fraction of recirculated exhaust gas in fresh charge
E_j	activation energy for forward rate constant, eq. (I-145)
E_m	mass of fresh charge divided by mass of residual exhaust gas, eq. (I-126)
$E^{(\pm)}_n$	$n=1, 2, 3, 4$ poppet valve flow parameters, eq. (I-117a)
$e^{(\pm)}$	poppet valve flow function, eq. (I-117a)
$\dot{e}$	eq. (I-66)
F_k	total volumetric force vector, eq. (I-5)
f_k	volumetric force vector, eq. (I-5)
g	Gibbs free energy per unit mass, eq. (I-130)
g_{kj}	metric tensor of three-dimensional space
$\dot{H}$	eq. (I-25) or eq. (I-62)
H^λ	partial molar enthalpy, eq. (I-134)
$^*H^\lambda$	enthalpy per mole of pure species λ
h	enthalpy per unit mass, eq. (I-131)
h_f	flame zone enthalpy
$\bar{h}$	heat transfer coefficient, eq. (I-105)
$\tilde{h}^{(\pm)}$	functions defined by eq. (I-122)

$\tilde{h}_1^{(-)}$	function defined by eq. (I-122)
$\tilde{h}_1^{(b)}$	function defined by eq. (I-123)
$\tilde{h}_2^{(b)}$	function defined by eq. (I-123)
$\dot{K}$	eqs. (I-27) or (I-64) and (I-76) or (I-77)
K_j	equilibrium constant, eqs. (I-140) and (I-144)
k	thermal conductivity of a mixture, eq. (I-153)
k_λ	thermal conductivity of pure species λ
$k_b(j\sigma)$	backward rate constant, eqs. (I-138) and (I-140)
$k_f(j\sigma)$	forward rate constant, eqs. (I-138) and (I-141)
$k_f(j)$	forward rate constant, eq. (I-145)
L	piston stroke
l	connecting rod length
$l^{(\pm)}$	valve lift
$l_0^{(\pm)}$	poppet valve flow parameter, eq. (I-117a)
M	mass contained in volume V, eq. (I-15), or as defined by eq. (I-37)
M_1	burned mass during combustion
M_2	unburned mass during combustion
M_b	burned mass function, eqs. (I-97), (I-101), and (I-104)
M_f	enflamed mass function, eqs. (I-92), (I-99), and (I-103)
$M^{(\pm)}$	$\int \dot{M}^{(\pm)}\,d\theta + c^{(\pm)}$, where $c^{(\pm)}$ are integration constants
$\dot{M}_b$	mass burning rate function, eqs. (I-97), (I-102), and (I-104)
$\dot{M}^{(\pm)}$	mass flow functions, eqs. (I-110) to (I-114)
$\mathfrak{M}$	mass flux through surface A
m	mass density
m_j^σ	third-body efficiency of species σ, eq. (I-141)
N	total number of species in a mixture
N_j	reaction parameter, equals N for third-body reactions and 1 for non-third-body reactions, eqs. (I-138) and (I-139)
N_R	number of distinct elementary reaction pairs, eq. (I-138)
$\dot{N}_\lambda$	eqs. (I-26) or (I-63) and (I-76) or (I-77)
n_j	parameter for forward rate constant, eq. (I-145), or exterior normal vector to a closed surface
n_λ	moles of species λ per unit mass
$n_\lambda^{(1)}$	moles of species λ per unit mass of burned gas
$n_\lambda^{(2)}$	moles of species λ per unit mass of unburned gas
$\tilde{n}_\lambda^{(\pm)}$	functions defined by eq. (I-121)
$\tilde{n}_\lambda^{(1,-)}$	function defined by eq. (I-121)
$n_\lambda^{(1,b)}$	function defined by eq. (I-123)
$n_\lambda^{(2,b)}$	function defined by eq. (I-123)
$n_\lambda^{(f)}$	moles of species λ per unit mass for flame zone
$\dot{P}$	eq. (I-65)
Pr	Prandtl number, eq. (I-106)
p	pressure
p_e	exhaust pressure
p_F	fuel pressure
p_f	flame zone pressure
p_m	manifold pressure

$(p_2/p_1)_c$	critical pressure ratio for poppet valve flow, eq. (I-115)
p^*	eq. (I-76)
p_1^*, p_2^*	eq. (I-77)
$p_{\bar{\mu}}^*$	volume flux average of pressure over a surface, eq. (I-30)
$\dot{Q}$	eqs. (I-24) or (I-61) and (I-76) or (I-77)
q^k	heat flux vector, eq. (I-1)
R	universal gas constant
R_λ	volumetric production rate for species λ, eqs. (I-3) and (I-143)
Re	Reynolds number for cylinder contents, eq. (I-107)
$\mathrm{Re}^{(\pm)}$	Reynolds number for flow through poppet valves, eq. (I-116)
r	compression ratio
r_0	cranking radius, $L/2$, eq. (I-84)
$r_n^{(\pm)}$	poppet valve flow parameters, eq. (I-117b)
S	volumetric production rate for ψ, eq. (I-13)
S^λ	symbol for chemical species λ, eq. (I-138), or partial molar entropy, eq. (I-134)
${}^*S^\lambda$	entropy per mole of pure species λ
s	entropy per unit mass, eq. (I-131)
T	absolute temperature
T_f	flame zone temperature
T_w	effective wall temperature
t	time
$t^{(\pm)}$	poppet valve thickness
U^λ	partial molar internal energy, eq. (I-134)
${}^*U^\lambda$	internal energy per mole of pure species λ
u	internal energy per unit mass
V	volume
V_1	volume occupied by burned mass during combustion
V_2	volume occupied by unburned mass during combustion
V^i	velocity vector characterizing displacement of a surface, eq. (I-8)
V^α	two-space velocity vector characterizing displacement of a curve on a surface, eq. (I-11)
V^λ	partial molar volume
v	velocity for use in calculation of heat transfer coefficient, eq. (I-108)
v_m	mean piston speed, $L\omega/\pi$
v_p	piston speed, eq. (I-109)
v^k	fluid velocity vector
W^α	two-space vector characterizing displacement of a curve on a surface, eq. (I-12)
$\mathcal{W}_\lambda$	molecular weight of species λ
w	fluid velocity normal to a surface, $v^i n_i$
x	piston displacement, eq. (I-84)
x^k	coordinates for three space, $k = 1, 2, 3$
y^α	coordinates of a two-dimensional subspace
z	$(\theta - \theta_0)/(\theta_f - \theta_0)$
α	parameter in Wiebe burning function, eqs. (I-99) and (I-101)
$\alpha^{(\pm)}$	parameter in expression for valve flow area, eq. (I-116)
β	parameter in Wiebe burning function, eqs. (I-99) and (I-101)
$\beta^{(\pm)}$	valve seat angles for poppet valves

Γ	$<v^2>/<w>^2$
γ	isentropic exponent, $(\partial \ln p/\partial \ln \rho)_s$
∇_k	covariant derivative
δ_{ij}	Kronecker delta
$\delta/\delta t$	convective differentiation operator, $\partial/\partial t + v^k \nabla_k$
ϵ	$L/2l$
η	shear viscosity of a mixture, eq. (I–152)
η_α	exterior normal to a closed curve on a surface
η_λ	shear viscosity of pure species λ
Θ	$v^2/2+\Omega$
θ	crankangle
θ_0	crankangle at start of combustion phase
θ_f	crankangle when all mass is enflamed
θ^*	crankangle at end of combustion phase
$\theta_o^{(\pm)}$	crankangle for intake or exhaust valve opening
$\theta_c^{(\pm)}$	crankangle for intake or exhaust valve closing
λ	$\pi\omega\tau/(\theta_f-\theta_0)$
μ^λ	chemical potential of species λ
$\hat{\mu}^\lambda$	internal energy transported by diffusion of one mole of species λ, eq. (I–1)
${}^*\mu^\lambda$	chemical potential of pure species λ at 1 atmosphere
$\nu_{\lambda j}$, $\nu'_{\lambda j}$	stoichiometric coefficients for non-third-body reactions, eq. (I–139)
$\nu_{\lambda j\sigma}$, $\nu'_{\lambda j\sigma}$	stoichiometric coefficients for reactions, eq. (I–138)
ρ	mean mass density, eq. (I–18) or (I–50)
σ	eq. (I–71)
$\sigma^{(\pm)}$	poppet valve flow function, eqs. (I–111) and (I–113)
τ	relaxation parameter for burning
τ^{kj}	stress tensor
$\Delta\tau^{kj}$	dissipative stress tensor
Φ	eq. (I–42)
φ	scalar field per unit volume
ϕ	one-parameter family of propagating surfaces
ψ	scalar field per unit mass
$\tilde{\psi}$	eq. (I–48)
$\tilde{\psi}_{\bar{\mu}}$	mass flux average of ψ over a surface, eqs. (I–31) and (I–36)
$\bar{\psi}^{(\pm)}$	eq. (I–120)
Ω	scalar force potential, eq. (I–5)
ω	angular velocity

Subscripts and superscripts:

b	flame zone burned-gas properties
e	exhaust properties
eq	equilibrium properties
$+$	intake system
$-$	exhaust system
0	fresh charge properties
1	burned gas, or upstream
2	unburned gas, or downstream

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Chapter II

Numerical Integration of Ordinary Differential Equations

Frank J. Zeleznik

The differential equations of Chapter I must be integrated if the hierarchy of models described there is to be utilitarian and not just a theoretical construct. Since analytical integration is out of the question, the integration must be accomplished numerically, and this then raises the problem of selecting a suitable integration scheme. Numerical integration of a system of ordinary differential equations is a numerical process for generating approximations to the true solution, at a number of discrete points, by replacing the system of differential equations with a system of ordinary equations. The numerical process not only generates approximations to the solution, but also produces estimates of some of its derivatives. A good numerical integration scheme must have two characteristics. First, it must be capable of producing an adequate approximation to the true solution. Second, it must generate the solution economically. The question of economy is a matter of concern when the system of equations is large. It is especially significant when some of the equations arise from chemical kinetic considerations. Differential equations associated with chemical kinetics sometimes exhibit a property called stiffness, which can reveal itself in the behavior of an integration algorithm. It takes excessively small steps, out of proportion to the rate of change of the dependent variables. Both of these considerations, accuracy and economy, apply to the systems of equations of Chapter I.

A broad spectrum of numerical integration algorithms for first order differential equations has been published in the literature. A significant fraction of these are methods which are classified as linear, multistep methods (ref. 1). A second category of methods is related to the Nordsieck method for integrating a system of first order differential equations, which first appeared in a 1962 paper by Nordsieck (ref. 2). The Nordsieck method of integrating a system of first order, ordinary, differential equations is a one-step, implicit method and its derivation was based on the use of a truncated Taylor series. Nordsieck pointed out (ref. 2, pp. 23 and 31) that his method can be thought of as a reformulation of Adams' linear, multistep method. Indeed, Gear (refs. 3 and 4) subsequently showed that there is a connection between the Nordsieck form of integration and the predictor-corrector process applied to first derivative, implicit, linear, multistep methods. In addition, Gear was able to extend Nordsieck's method to higher order differential equations (ref. 3). The extension of Nordsieck's method to higher order differential equations was also accomplished with somewhat different results by LaBudde (ref. 5). Gear (refs. 6 and 7) capitalized on a connection between the predictor-corrector multistep methods and the Nordsieck method to devise an integration scheme for systems of first order, stiff, differential equations. He incorporated both Nordsieck's reformulation of Adams' method and the Nordsieck-like version of his own stiff-equations method into a computer program (refs. 8 and 9) for first order differential equations which embodied automatic control of step size and integration order. An extensively modified and improved version of the Gear program has been developed by Hindmarsh (refs. 10 and 11). Commenting on Gear's stiff-equations method, Hull et al. find (ref. 12, p. 616) "it to be very efficient"; Gelinas states (ref. 13, p. 223) that it "fulfills the claims made of it"; while Enright writes (ref. 14, p. 322) that it "has become the most widely used method for stiff equations."

Because of the apparent success of the Nordsieck-like version of Gear's stiff-equations method it seems to be a logical starting point for the development of a suitable integration method for modeling the internal combustion engine. Numerical integration, like any other numerical calculation, is a blend of computational theory and computational art, with the art dependent to some degree on the theoretical understanding. As I have already mentioned, Gear developed his stiff-equations method through the theory of first derivative, linear, multistep methods. Yet, in application, the method is a one-step method with no vestiges of the linear, multistep methods. Hence it is desirable to establish the theory without recourse to linear, multistep methods, and that is precisely what I shall do. I shall obtain both Nordsieck's reformulation of Adams' method and the Nordsieck-like version of Gear's method for stiff equations as special cases of a new general class of integration formulas. These methods apply directly to first and higher order equations, which need not even be in normal form.

Some Exact Relations

Before defining and examining some of the properties of a general class of Nordsieck-like integration schemes, I wish to introduce some notation and to examine some exact relationships among derivatives which will motivate the definition of an extension of the Nordsieck method. I will be dealing with vector-valued functions defined on an interval of the reals, and in all cases the functions will be presumed to be n-dimensional vectors over the complex field. Suppose that $y(x)$ is such a function which possesses q derivatives and that $h \neq 0$ is real and represents the integration step size. If the conjugate transpose is denoted by an asterisk, then we can define an $n(q+1)$-dimensional vector η by

$$\eta^*(x, h, q) \equiv \left[\frac{h^0 y^{(0)*}(x)}{0!}, \frac{hy^{(1)*}(x)}{1!}, \ldots, \frac{h^q y^{(q)*}(x)}{q!}\right] \tag{II-1}$$

where $y^{(k)}(x)$ is the k^{th} derivative of $y(x)$. This vector characterizes the Nordsieck integration method, and the $(m+1)(q+1)n$-dimensional vector

$$\zeta^*(x, h, q, m) \equiv [\eta^*(x, h, q), \eta^*(x-h, h, q), \ldots, \eta^*(x-mh, h, q)] \tag{II-2}$$

characterizes all of the possible q^{th} derivative, linear, multistep methods of $m > 0$ steps. Of course, the dimensions of the vectors $\eta(x, h, q_1)$ and $\zeta(x, h, q_2, m)$ will be equal if and only if $q_1 + 1 = (m+1)(q_2+1)$, and obviously if $q_1 = q_2 = q$ and $m = 0$, then $\zeta(x, h, q, 0) = \eta(x, h, q)$.

I shall now establish some exact relationships between the vectors η and ζ. Suppose that $g(x)$ is a vector-valued function on an interval of the reals and possesses q derivatives. Then if l is an integer and both x and $x+lh$ are in the domain of g, we can define a remainder vector

$$r(l, q, x, h, g) \equiv g(x+lh) - \sum_{n=0}^{q} \frac{l^n h^n}{n!} g^{(n)}(x) \tag{II-3}$$

The remainder vector r clearly depends on l, q, x, h, and g, as the notation indicates. If g possesses a $(q+1)^{\text{th}}$ derivative, then r can be identified with $(h)^{q+1} g^{(q+1)}(\xi)/(q+1)!$, where ξ is some point in the open interval $(x, x+lh)$. In this case equation (II-3) becomes just the Taylor formula with the Lagrangian form of the remainder. Let us apply equation (II-3) to the vectors $h^s y^{(s)}(x)/s!$ for $s = 0$, $1, \ldots, q$. This immediately yields

$$\frac{h^s}{s!} y^{(s)}(x+lh) = \sum_{n=s}^{q} \binom{n}{s} \frac{l^{n-s} h^n}{n!} y^{(n)}(x) + r_s \qquad s = 0, 1, \ldots, q \tag{II-4}$$

where $\binom{n}{s} = n!/s!(n-s)!$ is the binomial coefficient and $r_s = r_s(l, q, x) \equiv r[l, q, x, h, h^s y^{(s)}(x)/s!]$ is the remainder associated with $h^s y^{(s)}(x)/s!$ when the expansion is terminated with the q^{th} derivative of y. If $y(x)$ is a polynomial of degree no greater than q, then r_s is zero for all s; for other functions it will generally be nonzero. We now define an upper triangular $(q+1)\times(q+1)$ matrix $P(l;q)$ by $P(0;q)=1_{q+1}$, where 1_{q+1} is the $(q+1)\times(q+1)$ identity matrix, and by

$$P_{ij}(l;q)=\begin{cases}\binom{j}{i}l^{j-i} & \text{for } i\leq j\\ \\ 0 & \text{for } j<i\end{cases}\qquad i, j=0, 1, 2, \ldots, q;\ l\neq 0 \tag{II-5}$$

and an $n(q+1)\times n(q+1)$ matrix $A(l;q)$ as the direct product of $P(l;q)$ and the $n\times n$ identity matrix 1_n.

$$A(l;q)\equiv P(l;q)\otimes 1_n=\begin{bmatrix} P_{00}(l;q)1_n & P_{01}(l;q)1_n & \ldots & P_{0q}(l;q)1_n\\ P_{10}(l;q)1_n & P_{11}(l;q)1_n & \ldots & P_{1q}(l;q)1_n\\ \\ \cdot & \cdot & \ldots & \cdot\\ \\ P_{q0}(l;q)1_n & P_{q1}(l;q)1_n & \ldots & P_{qq}(l;q)1_n\end{bmatrix}$$

Finally, if we define an $n(q+1)$-dimensional vector of remainders σ as

$$\sigma^*(l, q, x)\equiv\left[r_0^*(l, q, x), r_1^*(l, q, x), \ldots, r_q^*(l, q, x)\right] \tag{II-7}$$

then equation (II-4) translates into an exact expression for the propagation of the vector η from x to $x+lh$.

$$\eta(x+lh, h, q)=A(l;q)\eta(x, h, q)+\sigma(l, q, x) \tag{II-8}$$

This formula can now be used to write an exact expression for the propagation of ζ from x to $x+lh$. If we write

$$\tau^*(l, q, x, m)\equiv\left[\sigma^*(l, q, x), \sigma^*(l, q, x-h), \ldots, \sigma^*(l, q, x-mh)\right] \tag{II-9}$$

then from equations (II-2) and (II-8) we have

$$\zeta(x+lh, h, q, m)=\mathcal{A}(l, q, m)\zeta(x, h, q, m)+\tau(l, q, x, m) \tag{II-10}$$

where the $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix $\mathcal{A}(l, q, m)$ is just the direct sum of $m+1$ copies of $A(l;q)$.

$$\mathcal{A}(l, q, m)=1_{m+1}\otimes A(l;q) \tag{II-11}$$

The formula (II-4) also enables us to relate $\zeta(x, h, q_2, m)$ and $\eta(x, h, q_1)$. To express this concisely, we must make some additional definitions. Thus for $q_2\leq q_1$ we shall define a $(q_2+1)\times(q_1+1)$ submatrix $Q(l)$ of $P(l;q)$ as

$$Q(l)\equiv\begin{bmatrix} P_{00}(l;q_1) & P_{01}(l;q_1) & \ldots & P_{0q_1}(l;q_1)\\ P_{10}(l;q_1) & P_{11}(l;q_1) & \ldots & P_{1q_1}(l;q_1)\\ \\ \cdot & \cdot & \ldots & \cdot\\ \\ P_{q_20}(l;q_1) & P_{q_21}(l;q_1) & \ldots & P_{q_2q_1}(l;q_1)\end{bmatrix} \tag{II-12}$$

and the $(m+1)(q_2+1)\times(q_1+1)$ matrix Q as

$$Q^* \equiv \left[Q^*(0),\ Q^*(-1),\ \ldots,\ Q^*(-m)\right] \tag{II-13}$$

Simiarly we define an $n(m+1)(q_2+1)$-dimensional vector ρ.

$$\rho^*(q_2,\ x) \equiv \left[\sigma^*(0,\ q_2,\ x), \sigma^*(-1,\ q_2,\ x),\ \ldots,\ \sigma^*(-m,\ q_2,\ x)\right] \tag{II-14}$$

This notation permits us to write

$$\zeta(x,\ h,\ q_2,\ m) = (Q \otimes 1_n)\,\eta(x,\ h,\ q_1) + \rho(q_2,\ x) \tag{II-15}$$

Essentially equations (II-8), (II-10), and (II-15) are nothing more than the reexpression of the simple identity given as equation (II-4) and contain no new information. These three relations can still be further rewritten. Suppose v is an arbitrary vector which satisfies the condition $v^*v \neq 0$ and whose dimension is dim v. Then we can define an $n(q+1)\times \dim v$ matrix R and an $(m+1)(q+1)n \times \dim v$ matrix T as

$$\begin{aligned} R &\equiv \frac{\sigma v^*}{v^* v} \\ T &\equiv \frac{\tau v^*}{v^* v} \end{aligned} \tag{II-16}$$

and then $Rv = \sigma$, $Tv = \tau$, and equations (II-8) and (II-10) become

$$\begin{aligned} \eta(x+lh,\ h,\ q) &= A(l;q)\,\eta(x,\ h,\ q) + Rv \\ \zeta(x+lh,\ h,\ q,\ m) &= \mathcal{A}(l,\ q,\ m)\,\zeta(x,\ h,\ q,\ m) + Tv \end{aligned} \tag{II-17}$$

The second member of equation (II-17) will be the basis for a generalization of the Nordsieck method to be developed in the following section, and of course it reduces to the first member of equation (II-17) for $m=0$.

One more identity involving ζ and η, which complements the second member of equation (II-17), can be written. Let J_{m+1} be the $(m+1)\times(m+1)$ matrix with zeroes everywhere except ones above the main diagonal, that is,

$$J_{m+1} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ & \cdot & & \cdots & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix} \tag{II-18}$$

Thus $(J_{m+1})^{m+1} = 0$ and J_{m+1} is nilpotent of degree $m+1$. Then we can write the identity

$$\zeta(x+h,\ h,\ q,\ m) = \left[J^*_{m+1} \otimes 1_{n(q+1)}\right]\zeta(x,\ h,\ q,\ m) + \left[\eta^*(x+h,\ h,\ q), 0,\ \ldots,\ 0\right]^* \tag{II-19}$$

where the right side is a decomposition of the left side into orthogonal vectors which lie in different subspaces. The first $n(q+1)$ components of the first vector on the right side are zero, while the remaining components of the second vector are zero. This identity will enable us to give a concise expression for the conventional, linear, multistep methods so that these can then be contrasted with the general class of methods to be defined later.

The general class of integration methods will be designed to solve an initial-value problem associated with a p^{th} order ($p>0$) system of ordinary differential equations. Neither the initial values nor the form of the differential equations will be pertinent to most of the discussion of these integration methods. For this reason the allowed form of the differential equations is kept as broad as possible.

Definition I.1 Let $f[y^{(i)}(x),\ x]$ be a vector-valued function. Then $f[y^{(i)}(x),\ x]=0$ is said to be a p^{th} order differential equation for $y(x)$ if and only if $\partial f/\partial y^{(p)}\neq 0$ and $\partial f/\partial y^{(k)}=0$ for all $k>p$. If $f=0$ is a p^{th} order differential equation and $f=y^{(p)}-\varphi(y^{(0)},\ y^{(1)},\ \ldots,\ y^{(p-1)},\ x)$, then the differential equation is said to be in normal form.

Observe that in Definition I.1 there is no requirement that $f=0$ be explicitly solvable for $y^{(p)}$; that is, it need not be possible to actually write the differential equation in normal form.

Linear, Multistep Methods

I shall write the form of the most general q-derivative, linear, m-step method so that the form of these methods can later be compared with the general Nordsieck-like methods. The linear, multistep methods are based on the identity (II–19) and can only be used on first order equations in normal form. They are all of the form

$$Bz(x+h)=B\left(J^{*}_{m+1}\otimes 1_{n(q+1)}\right)z(x)+B\Big[y^{*}(x+h),\ h\varphi^{*}(x+h),\ \frac{h^{2}\varphi^{(1)*}(x+h)}{2!},\ \ldots,$$

$$\frac{h^{q}\varphi^{(q-1)*}(x+h)}{q!},\ 0,\ldots,\ 0\Big]^{*}=0 \qquad \text{(II–20)}$$

where $z(x)$ is an approximation to $\zeta(x,\ h,\ q,\ m)$, B is an $n\times n(m+1)(q+1)$ matrix which has the form

$$B=\left(B_{1},\ B_{2},\ \ldots,B_{(m+1)(q+1)}\right) \qquad \text{(II–21)}$$

where B_i are $n\times n$ matrices, and the differential equation is $y^{(1)}=\varphi(y,\ x)$. Equation (II–20) is viewed as an equation for a hopefully unique $y(x+h)$ and the matrices B_i are constrained by the requirement that equation (II–20) be exact for all polynomials of degree less than some given degree. Most often the multistep methods are first derivative methods ($q=1$) although second derivative methods ($q=2$) are known and these are discussed by Enright (ref. 14). Almost universally the matrices B_i are chosen to be constant scalar matrices. That is, B is written as

$$B=(\alpha_{0},\ \beta_{0},\ \gamma_{0},\ \ldots,\ \alpha_{1},\ \beta_{1},\ \gamma_{1},\ \ldots,\ \alpha_{m},\ \beta_{m},\ \gamma_{m},\ \ldots)\otimes 1_{n}$$

where the α_i, β_i, γ_i, . . . are constants. The class of methods for which all α_i, γ_i, . . . are zero except $\alpha_0=1$ and $\alpha_1=-1$ are known as Adams' methods. The simplest of these, $\beta_0=1/2$, $\beta_1=-1/2$, and $\beta_i=0$ for $i>1$, is also known as the Euler method. Lambert and Sigurdsson (ref. 15) look at first derivative methods with variable, nonscalar matrices. Some of the matrices B_i will be zero in a particular linear, multistep method, and hence the corresponding part of the vector z is annihilated by B. Suppose we define a characteristic function $\theta(i)$ by

$$\theta(i) = \begin{cases} 1 & B_i = 0 \\ 0 & B_i \neq 0 \end{cases} \tag{II-22}$$

and an $\left[(m+1)(q+1) - \sum_k \theta(k)\right] \times (m+1)(q+1)$ matrix Ψ by the prescription

$$\Psi_{ij} = \begin{cases} 1 & i = j - \sum_{k=1}^{j} \theta(k) \text{ and } B_j \neq 0 \\ 0 & \text{otherwise} \end{cases} \tag{II-23}$$

where i has the range $1 \leq i \leq (m+1)(q+1) - \sum_{k=1}^{(m+1)(q+1)} \theta(k)$ and j has the range $1 \leq j \leq (m+1)(q+1)$. Then any particular linear, multistep method is characterized not by ζ but actually by $(\Psi \otimes 1_n)\zeta$ because $\Psi \otimes 1_n$ annihilates noncontributing components. When equation (II-15) is multiplied by the matrix $\Psi \otimes 1_n$, we obtain

$$(\Psi \otimes 1_n)\zeta(x,\ h,\ q_2,\ m) = \left[(\Psi Q) \otimes 1_n\right]\eta(x,\ h,\ q_1) + (\Psi \otimes 1_n)\rho(q_2,\ x) \tag{II-24}$$

If ψQ is nonsingular, then this equation can be solved for η and the Nordsieck method, characterized by $\eta(x,\ h,\ q_1)$, can be thought of as being equivalent, in some sense, to the linear, multistep method characterized by $(\Psi \otimes 1_n)\zeta(x,\ h,\ q_2,\ m)$. Obviously they cannot be thought of as numerically equivalent since the relationship (II-24) in no way takes into account either the effect of the nonzero B_i or the details of the Nordsieck method. Certainly a necessary condition for ΨQ to be nonsingular is that it be a square matrix. That is, it is necessary that

$$q_1 + 1 = (m+1)(q_2+1) - \sum_{k=1}^{(m+1)(q_2+1)} \theta(k)$$

Gear (refs. 6 and 7) used equation (II-24) with special cases of ΨQ to convert the predictor-corrector versions of his stiffly stable, linear, multistep methods into a Nordsieck form.

A concise derivation of Gear's connection (refs. 3 and 4) between predictor-corrector, first derivative, linear, multistep methods and the Nordsieck form is easily given with the more general framework established by equation (II-20). The linear, multistep method, equation (II-20), with $q=1$, takes the form

$$\omega \equiv B_1 y(x+h) + B_2 h\varphi\left[y(x+h),\ x+h\right] + W(x) = 0$$

$$W(x) \equiv B(J^*_{m+1} \otimes 1_{2n}) z(x) \tag{II-25}$$

for a first order differential equation in normal form. The equation $\omega = 0$ is to be regarded as an equation for $y(x+h)$. Its iterative solution by the Newton method takes the form

$$\omega^{(i)} + J^{(i)} \Delta y^{(i)} = 0 \tag{II-26}$$

where

$$J \equiv \frac{\partial \omega}{\partial y} = B_1 + hB_2 K$$

$$K \equiv \frac{\partial \varphi}{\partial y}$$

$$\Delta y^{(i)} \equiv y^{(i+1)} - y^{(i)}$$

and where both B_1 and B_2 are presumed to be independent of x and y. These equations immediately imply

$$-\left(J^{(i)} \Delta y^{(i)} - J^{(i-1)} \Delta y^{(i-1)}\right) = \omega^{(i)} - \omega^{(i-1)} = B_1\ \Delta y^{(i-1)} + hB_2\left(\varphi^{(i)} - \varphi^{(i-1)}\right)$$

where now $\varphi^{(i)}$ is the i^{th} estimate of φ, not its i^{th} derivative, and thus

$$\begin{aligned}-J^{(i)} \Delta y^{(i)} &= -\left(J^{(i-1)} - B_1\right) \Delta y^{(i-1)} + hB_2\left(\varphi^{(i)} - \varphi^{(i-1)}\right) \\ &= B_2\left(h\varphi^{(i)} - hK^{(i-1)} \Delta y^{(i-1)} - h\varphi^{(i-1)}\right)\end{aligned}$$

If we define, for $i>0$, a vector $d^{(i)}$ by

$$d^{(i)} \equiv h\varphi^{(i-1)} + hK^{(i-1)} \Delta y^{(i-1)} \tag{II-27}$$

then the equation for $\Delta y^{(i)}$ becomes

$$J^{(i)} \Delta y^{(i)} = -B_2\left(h\varphi^{(i)} - d^{(i)}\right) \tag{II-28}$$

From equations (II-27) and (II-28) it follows that

$$\begin{aligned}d^{(i+1)} &= h\varphi^{(i)} + hK^{(i)} \Delta y^{(i)} \\ &= h\varphi^{(i)} + hK^{(i)} \left(J^{(i)}\right)^{-1} J^{(i)} \Delta y^{(i)} \\ &= h\varphi^{(i)} - B_2^{-1}\left(J^{(i)} - B_1\right)\left(J^{(i)}\right)^{-1} B_2\left(h\varphi^{(i)} - d^{(i)}\right) \\ &= h\varphi^{(i)} - \left[1_n - B_2^{-1} B_1 \left(J^{(i)}\right)^{-1} B_2\right]\left(h\varphi^{(i)} - d^{(i)}\right)\end{aligned}$$

and this provides a simple equation for the change of the vector d during iteration.

$$\Delta d^{(i)} \equiv d^{(i+1)} - d^{(i)} = B_2^{-1} B_1 \left(J^{(i)}\right)^{-1} B_2\left(h\varphi^{(i)} - d^{(i)}\right)$$

Since $J^{-1} = \left(1_n + B_1^{-1} B_2 hK\right)^{-1} B_1^{-1}$ it follows that $J^{-1} B_2 = \left(1_n + hB_1^{-1} B_2 K\right)^{-1} \left(B_2^{-1} B_1\right)^{-1}$ and $B_2^{-1} B_1 J^{-1} B_2 = \left(B_2^{-1} B_1\right) \left(1_n + hB_1^{-1} B_2 K\right)^{-1} \left(B_2^{-1} B_1\right)^{-1}$. From these expressions it is easily shown that $B_2^{-1} B_1 J^{-1} B_2 = \left(1_n + hB_1^{-1} B_2 K\right)^{-1}$ and $J^{-1} B_2 = B_1^{-1} B_2 \left(1_n + hB_1^{-1} B_2 K\right)^{-1}$ if and only if $(B_2^{-1} B_1) K = K\ (B_2^{-1} B_1)$. Hence when this commutation condition on the matrices holds, the equations for $\Delta y^{(i)}$ and $\Delta d^{(i)}$ are very similar.

$$\begin{aligned}\Delta y^{(i)} &= -\left(B_1^{-1} B_2\right)\left(1_n + hB_1^{-1} B_2 K^{(i)}\right)^{-1}\left(h\varphi^{(i)} - d^{(i)}\right) \\ \Delta d^{(i)} &= (1_n)\left(1_n + hB_1^{-1} B_2 K^{(i)}\right)^{-1}\left(h\varphi^{(i)} - d^{(i)}\right)\end{aligned} \tag{II-29}$$

From these equations for $\Delta y^{(i)}$ and $\Delta d^{(i)}$ it follows that $\Delta y^{(i)}=0$ if and only if $h\varphi^{(i)}-d^{(i)}=0$ if and only if $\Delta d^{(i)}=0$. This leads to the interpretation of $d^{(i)}$ as the i^{th} estimate for $hy^{(1)}(x+h)$ with convergence of $d^{(i)}$ to $h\varphi[y(x+h), x+h]$. The initial estimate, $d^{(0)}$, is still undefined since the definition of $d^{(i)}$ given in equation (II-27) is meaningless for $i=0$. But obviously $d^{(0)}$ should be so chosen that the $i=0$ versions of equations (II-26) and (II-28) agree if the iteration is to converge to a solution of equation (II-25).

$$-\omega^{(0)}=J^{(0)}\,\Delta y^{(0)}=-B_2\left(h\varphi^{(0)}-d^{(0)}\right)$$

This then gives a value for the initial estimate $d^{(0)}$.

$$\begin{aligned}d^{(0)}&=h\varphi^{(0)}-B_2^{-1}\omega^{(0)}\\&=h\varphi^{(0)}-B_2^{-1}\left(B_1y^{(0)}+B_2h\varphi^{(0)}+W(x)\right)\\&=-B_2^{-1}\left(B_1y^{(0)}+W(x)\right)\\&=-B_2^{-1}\left[B_1y^{(0)}+B\left(J_{m+1}^{*}\otimes 1_{n(q+1)}\right)z(x)\right]\end{aligned}\tag{II-30}$$

Suppose we define

$$\left(\bar{z}^{(i)}\right)^{*}=\left\{y^{(i)*}, d^{(i)*}, y^{*}(x), h\varphi^{*}(x), \ldots, y^{*}[x-(m-1)h], h\varphi^{*}[x-(m-1)h]\right\}^{*}$$

then $\bar{z}^{(i)}$ will converge to $z(x+h)$ when $d^{(0)}$ is chosen as in equation (II-30) and, using equation (II-29), the iteration can be written as

$$\Delta\bar{z}^{(i)}\equiv\bar{z}^{(i+1)}-\bar{z}^{(i)}=\left[-\left(B_1^{-1}B_2\right)^{*}, 1_n, 0, \ldots, 0\right]^{*}\left(1_n+hB_1^{-1}B_2K^{(i)}\right)\left(h\varphi^{(i)}-d^{(i)}\right)\tag{II-31}$$

Since $\bar{z}(x+h)$ is regarded as an approximation for $\zeta(x+h, h, q_2=1, m)$, it follows from equation (II-24) that

$$\begin{aligned}\left[(\Psi Q)^{-1}\otimes 1_n\right]\Delta\bar{z}^{(i)}&=\left[(\Psi Q)^{-1}\otimes 1_n\right]\\&\quad\times\left[-\left(B_1^{-1}B_2\right)^{*}, 1_n, 0, \ldots, 0\right]^{*}\left(1_n+hB_1^{-1}B_2K^{(i)}\right)\left(h\varphi^{(i)}-d^{(i)}\right)\end{aligned}\tag{II-32}$$

can be regarded as the Nordsieck form of the same iterative calculation. Equation (II-32) is the generalization of Gear's results, which were obtained by him for the special case where the matrices B_i are scalar matrices. The commutation condition clearly holds for scalar matrices.

Several observations should be made about the results given as equations (II-31) and (II-32). First, the iteration (II-31) directly involves only the matrices B_1 and B_2; the remaining submatrices of B appear only in the definition of $d^{(0)}$. Second, the iterations for y and d are not independent because $d^{(0)}$ is defined in terms $y^{(0)}$ in equation (II-30) and this establishes an interaction. If the iteration (II-31) converges, it will converge to a solution of equation (II-25) if and only if $d^{(0)}$ is chosen as in equation (II-30). Any other choice, say $\bar{d}^{(0)}$, is equivalent to replacing $W(x)$ in the first member of equation (II-25) with

$$\overline{W}(x)=W(x)+B_2\left(d^{(0)}-\bar{d}^{(0)}\right)=-B_1y^{(0)}-B_2\bar{d}^{(0)}$$

and this effectively redefines the linear, multistep method. Finally the derivation of equation (II-32) is valid only for first order equations in normal form. A similar derivation is not possible for higher order differential equations.

The implementation of linear, multistep integration methods for first order equations in the Nordsieck form (eq. (II–32)) with B_i as scalar matrices, both by Gear (refs. 8 and 9) and by Hindmarsh (refs. 10 and 11) differs significantly from the conditions necessary for its derivation. First, $(h\varphi^{(n)} - d^{(n)})$ was reinterpreted as the differential equation multiplied by h, $h(\varphi - dy/dx)$, evaluated with the n^{th} estimates for y and dy/dx. Second, the initial estimates for y and dy/dx did not satisfy the constraint (II–30) necessary for the derivation. Consequently the implemented algorithm is not the algorithm which was theoretically analyzed. The difference between the implemented algorithm and the analyzed algorithm is further increased because the transformation (II–24) from linear, multistep form to Nordsieck form is only exact when the contribution from remainders ρ is known. The remainders are never known in practice. The method was extended to higher order differential equations (ref. 3) by the *ad hoc* procedure of assuming that the first order equation can be replaced by a p^{th} order differential equation multiplied by $h^p/p!$.

The lacuna between theory and practice suggests that a broader look at the Nordsieck-like integration method is in order. One of the goals of such an investigation should be the construction of a large class of integration formulas which contain, as special cases, both Nordsieck's reformulation of Adams' method and the Nordsieck-like version of Gear's method for stiff equations. Another goal should be an examination of the stability characteristics of this class of integration formulas. A third goal should be the establishment of the degree of freedom that is available in the choice of the parameters which characterize a particular method of the general class. The analysis to achieve these goals is described in the following sections.

General Class of Nordsieck-Like Methods

Before defining a generalization of the Nordsieck integration method I must first introduce some notation. If we define the nonsingular matrix

$$H \equiv \operatorname{diag}\left(\frac{h^0}{0!}, \frac{h}{1!}, \ldots, \frac{h^q}{q!}\right) \otimes 1_n \tag{II-33}$$

then we can write $\eta = H\xi$, where

$$\xi^* \equiv [y^{(0)*}, y^{(1)*}, \ldots, y^{(q)*}]$$

Hence any function $f[y^{(i)}, x]$ can also be regarded as a function of η and so, with traditional abuse of notation, I shall sometimes use $f(\eta, x)$ instead of $f(y^{(i)}, x) = f(\xi, x)$. Keeping this in mind, we can now write a generalization of Nordsieck's method. The generalization is based on the form of the second member of equation (II–17).

Definition I.2 Let $f = 0$ be a p^{th} order differential equation, where $0 < p \leq q$ and where p and q are integers. Furthermore, let $M = M(x, h, q, m)$ and $N = N(x, h, q, m)$ be $(m+1)(q+1)n \times (m+1)n$ matrices and $F(\zeta, x)$ be the $(m+1)n$-dimensional vector defined as $F^*(\zeta, x) = \{f^*[\eta(x), x], f^*[\eta(x-h), x-h], \ldots, f^*[\eta(x-mh), x-mh]\}$. The general (M, N)-Nordsieck integration method of polynomial degree q and $m+1$ steps associated with $f(\eta, x) = 0$ is defined by $z(x+h) = \mathcal{Q}(q, m)z(x) + Nz_{q+1}$, where $\mathcal{Q}(q, m) \equiv \mathcal{Q}(1, q, m)$, and z_{q+1} is a vector of dimension $(m+1)n$ and is defined to be a solution of $F(w, x+h) = 0$ where $w \equiv \mathcal{Q}(q, m)z(x) + Mz_{q+1}$.

Some observations can be made immediately about the general integration method of Definition I.2. It, like all numerical integration schemes, replaces the integration process by the process of solving a system of equations. Generally speaking, the equations to be solved are nonlinear and the method is viable only so long as $F = 0$ possesses a solution, hopefully unique, for z_{q+1}. A comparison of Definition I.2 with equation (II–17) discloses that Nz_{q+1} can be thought of as a direct measure of the truncation error. The vector $z(x)$ represents the method's approximation to $\zeta(x)$, and this suggests that $z(x)$ be partitioned in a manner identical to the partitioning of $\zeta(x)$ in equation (II–2).

$$z^*(x) = \left[a^*(x),\ a^*(x-h),\ \ldots,\ a^*(x-mh)\right] \tag{II-34}$$

The vector $a(x)$ serves as the approximation to $\eta(x)$, and this in turn suggests that it be partitioned in a manner analogous to the partitioning of $\eta(x)$ in equation (II-1).

$$a^*(x) = \left[a_0^*(x),\ a_1^*(x),\ \ldots,\ a_q^*(x)\right] \tag{II-35}$$

Hence $i!h^{-i}a_i(x)$ plays the role of an approximation to the i^{th} derivative of a solution of $f=0$ at the point x. The method does not require $z(x)$ to satisfy the differential equations $f=0$ at the $m+1$ points $x,\ x-h,\ \ldots,\ x-mh$ in the sense that it does not require $F[z(x),\ x]=0$. However, w certainly does satisfy the differential equations at the $m+1$ points $x+h,\ x,\ \ldots,\ x-(m-1)h$. Since $z(x+h)-w=(N-M)z_{q+1}$, we know that if $(N-M)z_{q+1}=0$, then $z(x+h)=w$ and $F[z(x+h),\ x+h]=0$, and thus $z(x+h)$ satisfies the differential equations. This condition can always be satisfied, at least by the choice $M=N$, and so, in principle, it is always possible to generate a vector z which satisfies $f=0$ at $m+1$ points in one step of the calculation. This is important because numerical calculations are never exact and, as a result, we cannot expect $F[z(x),\ x]$ to be exactly zero for any x. The requirement that $F[z(x+h),\ x+h]=0$ can be viewed as a mechanism not only for obtaining an approximation to $\eta(x+h)$, but also for refining the approximations to η at previous points. The methods of Definition I.2 offer a number of features that are unavailable in the usual linear, multistep methods:

(1) They are directly applicable to p^{th} order differential equations of arbitrary form.
(2) They allow improvements to previous estimates of $\eta(x)$.
(3) They supply a direct measure of the truncation error.

The implementation of any integration method must deal with two questions: one concerning the method of solving the associated system of equations, and the other concerning the stability of the integration method. The former, on the one hand, is only peripherally related to the integration method in the sense that any method which provides a solution can be used to implement the integration scheme and the results, at least in principle, are independent of the solution technique. The solution method is patently a factor in practice, of course. Stability, on the other hand, is a characteristic of the method, and the calculated results might be strongly dependent on the stability properties. For these reasons a study of the stability of the methods of Definition I.2 will be given in the next section, while the solution of the equations will be given only a cursory look in the remainder of this section. A large class of iterative solution methods can be written in the form

$$\begin{aligned} z_{q+1}^{(k+1)} &= z_{q+1}^{(k)} + \Delta z_{q+1}^{(k)} \\ z^{(k+1)}(x+h) &= z^{(k)}(x+h) + N\,\Delta z_{q+1}^{(k)} \end{aligned} \tag{II-36}$$

where $z_{q+1}^{(k)}$ is the k^{th} approximation to z_{q+1} and $\Delta z_{q+1}^{(k)}$ is the solution of

$$J^{(k)}\Delta z_{q+1}^{(k)} = -\lambda^{(k)}F^{(k)} \tag{II-37}$$

In this equation $J^{(k)}$ is some nonsingular $n(m+1)\times n(m+1)$ matrix, $\lambda^{(k)}$ is an iteration step-size controlling parameter, and $F^{(k)}=F[w^{(k)},\ x+h]$, where $w^{(k)}$ is the k^{th} approximation to w; that is $w^{(k)}=\mathcal{A}(q,\ m)z(x)+Mz_{q+1}^{(k)}$. The choices $J^{(k)}=1_{n(m+1)}$, $\lambda^{(k)}=1$ give the successive substitutions iteration which is so often used to solve the nonlinear equations associated with the linear, multistep methods. In that application it produces the conventional predictor-corrector schemes. The choices $J^{(k)}=\beta^{(k)}M$, $\lambda^{(k)}=1$ give Newton's iteration if the $n(m+1)\times(m+1)(q+1)n$ matrix $\beta^{(k)}$ is

$$\beta^{(k)} \equiv \left.\frac{\partial F(\zeta,\ x+h)}{\partial \zeta}\right|_{\zeta=w^{(k)}} = \frac{\partial F(w^{(k)},\ x+h)}{\partial w^{(k)}} \tag{II-38}$$

If $J^{(k)}$ is initially calculated as for Newton's method but not altered for subsequent iterations, then we have the modified Newton method. Suppose that w is partitioned in the manner of z (eq. (34)).

$$w^* = \left(w_0^*,\ w_1^*,\ \ldots,\ w_m^*\right) \tag{II-39}$$

and we define an $n \times n(q+1)$ matrix for each α as

$$\beta_\alpha^{(k)} \equiv \left.\frac{\partial f(\eta,\ x+h-\alpha h)}{\partial \eta}\right|_{\eta = w_\alpha^{(k)}} = \frac{\partial f\left(w_\alpha^{(k)},\ x+h-\alpha h\right)}{\partial w_\alpha^{(k)}} \qquad \alpha = 0,\ 1,\ 2,\ \ldots,\ m \tag{II-40}$$

Then $\beta^{(k)}$ can be regarded as the direct sum of the $m+1$ matrices $\beta_\alpha^{(k)}$.

$$\beta^{(k)} = \oplus \sum_{\alpha=0}^{m} \beta_\alpha^{(k)} \tag{II-41}$$

There are, of course, other possible choices for $J^{(k)}$. For any choice, it is necessary to solve equation (II-37) for $\Delta z_{q+1}^{(k)}$. In practice this is achieved most economically by a direct solution (ref. 16) although there may exist special situations where one might wish to solve for $\Delta z_{q+1}^{(k)}$ by inverting $J^{(k)}$.

Regardless of which iterative method is used to solve for z_{q+1} one must be careful not to ascribe deficiencies of the solution technique to the integration method. To point up this fact, and to illustrate the integration method, let us look at the most general system of linear equations since the calculations can be carried out analytically for this case. Thus we take

$$f = \sum_{i=0}^{q} D_i(x) y^{(i)} + g(x) \tag{II-42}$$

where the $n \times n$ matrices D_i and the n-dimensional vector g are functions of x alone. We can define matrices β and β_α analogously to the definitions of $\beta^{(k)}$ and $\beta_\alpha^{(k)}$.

$$\beta \equiv \frac{\partial F(w,\ x+h)}{\partial w} \tag{II-43}$$

$$\beta_\alpha \equiv \frac{\partial f(w_\alpha,\ x+h-\alpha h)}{\partial w_\alpha} \qquad \alpha = 0,\ 1,\ 2,\ \ldots,\ m \tag{II-44}$$

and then

$$\beta = \oplus \sum_{\alpha=0}^{m} \beta_\alpha \tag{II-45}$$

For the linear function (II-42) we find

$$F(\zeta,\ x+h) = \beta\zeta + G \tag{II-46}$$

$$F(w,\ x+h) = \beta w + G = \beta \mathfrak{A} z(x) + \beta M z_{q+1} + G \tag{II-47}$$

where

$$G^* = \left[g^*(x+h),\ g^*(x),\ \ldots,\ g^*(x+h-mh)\right] \tag{II-48}$$

and

$$\beta_\alpha=\beta_\alpha^{(k)}=\left[h^{-0}0!D_0(x+h-\alpha h),\ h^{-1}1!D_1(x+h-\alpha h),\ \ldots,\ h^{-q}q!D_q(x+h-\alpha h)\right] \tag{II-49}$$

From equation (II–47) it is obvious that a unique solution exists for z_{q+1} if and only if βM is nonsingular and then

$$z_{q+1}=-(\beta M)^{-1}[\beta\mathfrak{A}z(x)+G] \tag{II-50}$$

$$z(x+h)=\left[1_{(m+1)(q+1)n}-N(\beta M)^{-1}\beta\right]\mathfrak{A}z(x)-N(\beta M)^{-1}G \tag{II-51}$$

$$F[z(x+h),\ x+h]=\beta z(x+h)+G=\left[1_{(m+1)n}-\beta N(\beta M)^{-1}\right][\beta\mathfrak{A}z(x)+G] \tag{II-52}$$

The vector $\beta\mathfrak{A}z(x)+G$ cannot generally be expected to equal the zero vector and hence, at least for linear problems, we find $F[z(x+h),\ x+h]=0$ for all linear problems if and only if $\beta(M-N)=0$. This is less restrictive than the condition $M=N$.

The question now is what would an iterative solution produce as the answer to the same problem. To permit an exact calculation, let us suppose that $\lambda^{(k)}$ and $J^{(k)}$ in equation (II–37) are independent of the iteration number k, and hence we write using equation (II–47)

$$\Delta z_{q+1}^{(k)}=-\lambda J^{-1}F^{(k)}=-\lambda J^{-1}\left[\beta\mathfrak{A}z(x)+\beta Mz_{q+1}^{(k)}+G\right]$$

and so

$$z_{q+1}^{(k+1)}=z_{q+1}^{(k)}+\Delta z_{q+1}^{(k)}=\left[1_{(m+1)n}-\lambda J^{-1}\beta M\right]z_{q+1}^{(k)}-\lambda J^{-1}[\beta\mathfrak{A}z(x)+G]$$

Since for the problem under consideration the matrix multiplying $z_{q+1}^{(k)}$ is independent of k, we find

$$z_{q+1}^{(k)}=\left(1_{(m+1)n}-\lambda J^{-1}\beta M\right)^k z_{q+1}^{(0)}-\sum_{l=0}^{k-1}\left[1_{(m+1)n}-\lambda J^{-1}\beta M\right]^l\lambda J^{-1}[\beta\mathfrak{A}z(x)+G] \tag{II-53}$$

If C is any square matrix, then

$$\lim_{k\to\infty} C^k=0$$

$$(1-C)^{-1}=\sum_{l=0}^{\infty}C^l$$

if and only if the spectral radius of C is less than 1 (ref. 17). From this it follows that

$$\sum_{l=0}^{k-1}C^l=(1-C)^{-1}(1-C^k)$$

Thus if the spectral radius of $1_{(m+1)n}-\lambda J^{-1}\beta M$ is less than 1, we find

$$z_{q+1}^{(k)}=\left[1_{(m+1)n}-\lambda J^{-1}\beta M\right]^k z_{q+1}^{(0)}-(\lambda J^{-1}\beta M)^{-1}$$

$$\times\left[1_{(m+1)n}-\left(1_{(m+1)n}-\lambda J^{-1}\beta M\right)^k\right]\lambda J^{-1}[\beta\mathfrak{A}z(x)+G] \tag{II-54}$$

and in the limit $k\to\infty$

$$z_{q+1}^{(\infty)}=-(\lambda J^{-1}\beta M)^{-1}\lambda J^{-1}[\beta\mathfrak{A}z(x)+G]$$

Newton's iteration gives the exact answer to a linear problem in one step. Thus the choice $\lambda = 1$, $J = \beta M$ in equation (II–54) gives $z_{q+1}^{(1)} = z_{q+1}^{(\infty)} = z_{q+1}$. For the successive-substitutions iteration $\lambda = 1$, $J = 1_{(m+1)n}$ and we find that

$$z_{q+1}^{(k)} = \left[1_{(m+1)n} - \beta M\right]^k z_{q+1}^{(0)} - (\beta M)^{-1}\left[1_{(m+1)n} - \left(1_{(m+1)n} - \beta M\right)^k\right]\left[\beta \mathcal{A} z(x) + G\right]$$

but $z_{q+1}^{(k)} \neq z_{q+1}^{(\infty)} = z_{q+1}$ and all of this is predicated on $1_{(m+1)n} - \beta M$ having a spectral radius less than 1. This is equivalent to requiring βM to have a spectral radius in the open interval (0,2), which might or might not be satisfied in any given problem. Here we have an example of an iterative method which could diverge or produce a poor approximation for z_{q+1}, and hence also for $z(x+h)$, even though a unique solution exists. It is imperative that one obtain the correct solution, or at least an adequate approximation to the solution, of the nonlinear equations when it exists. Failing this risks imputing inadequacies of the solution technique to the integration method. Certainly the efficacy of a particular algorithm is a combination of the two factors.

Stability

The stability of an integration method generally refers to its behavior when applied to a particular class of linear differential equations and not to the intuitive notion of how errors propagate during the numerical solution of the differential equations in general. Thus Lambert and Sigurdsson (ref. 15, p. 721) introduce $\bar{A}$ stability for the special case of equation (II–42) corresponding to the choice D_0 equal to a constant matrix, $-D_1 = 1_n$, $D_{i \geq 2} = 0$, and $g(x) = 0$. If D_0 is chosen as a constant scalar matrix, then $\bar{A}$ stability reduces to Dahlquist's A stability (ref. 18, p. 29). Prothero and Robinson (ref. 19, p. 147) introduce S stability for the special case where D_0 is equal to a constant matrix, $-D_1 = 1_n$, $D_{i \geq 2} = 0$, and $g(x) = -(D_0 u + du/dx)$, where u is a known function and $n = 1$. Because of the relative simplicity of the methods of Definition I.2, it will be unnecessary to use any of these arbitrary definitions of stability. Instead we can analyze the situation more generally without recourse to special differential equations. From Definition I.2 it follows that the variation $\delta z(x+h)$ in $z(x+h)$ can be expressed in terms of the variations $\delta z(x)$, δz_{q+1} in $z(x)$ and z_{q+1}. The same holds true for the variation $\delta F(w, x+h)$ of $F(w, x+h)$.

$$\begin{aligned} &\delta z(x+h) = \mathcal{A}\delta z(x) + N\delta z_{q+1} \\ &\delta F(w, x+h) = \beta\delta w = \beta\left[\mathcal{A}\delta z(x) + M\delta z_{q+1}\right] \end{aligned} \tag{II-55}$$

If βM is nonsingular, then the second of these can be used to eliminate δz_{q+1} from the first equation to give

$$\delta z(x+h) = S\delta z(x) + N(\beta M)^{-1}\delta F \tag{II-56}$$

where

$$S \equiv \left[1_{(m+1)(q+1)n} - N(\beta M)^{-1}\beta\right]\mathcal{A} \tag{II-57}$$

Thus the stability matrix S controls the propagation of errors in the initial values $z(x)$, while the matrix $N(\beta M)^{-1}$ controls the propagation of errors due to poor solutions of $F(w, x+h) = 0$. In principle, it is possible to achieve $\delta F = 0$, but in practice this will seldom be true. Hence the error at $x+h$ will contain contributions from both terms. However, let us suppose that $\delta F = 0$ and that S is independent of x. Then $\delta z(x+kh) = S^k \delta z(x)$ and thus, if $\delta z(x)$ is regarded as arbitrary, we conclude that $\delta z(x+kh) = 0$ if and only if $S^k = 0$. Obviously errors in $z(x)$ will propagate for a finite number of steps, less than or equal to k. If S is not nilpotent of degree k, then there still exists the possibility that $S^k \to 0$ as $k \to \infty$, which is true if the spectral radius of S is less than 1 (ref. 17). As a minimum then,

S should have its eigenvalues within the unit circle. The only freedom available for adjusting the eigenvalues of S is furnished by the matrices M and N, and so we shall begin an examination of the relationship of S to these matrices.

There are two ways in which we might proceed. We could, in effect, choose M and N and then ask what are the eigenvalues of S. This will not be considered in this report. Alternatively we might choose S and ask for the matrices M and N which produced it. This question will be examined for the balance of this section, and in the course of the discussion we will make use of the properties of the generalized (Moore-Penrose) inverse $M^\dagger$ of a matrix M. The definition and the necessary properties of generalized inverses are summarized in the appendix to this chapter. The subscript on the identity matrix will be suppressed on the following pages; that is, the $n \times n$ identity matrix 1_n will simply be written as 1, as will every other identity matrix.

Theorem II.1 The equation $S=[1-X\beta]\mathfrak{A}$ possesses a solution for X if and only if S is of the form $S=(1-Y_1\beta^\dagger\beta)\mathfrak{A}$. The solution is $X=(1-S\mathfrak{A}^{-1})\beta^\dagger+Y_2(1-\beta\beta^\dagger)=Y_1\beta^\dagger+Y_2(1-\beta\beta^\dagger)$, where Y_1 and Y_2 are arbitrary matrices such that Y_1 is $(m+1)(q+1)n\times(m+1)(q+1)n$ and Y_2 is $(m+1)(q+1)n\times(m+1)n$.

Proof: Clearly from the properties of the generalized inverse, $X\beta=[Y_1\beta^\dagger+Y_2(1-\beta\beta^\dagger)]\beta=Y_1\beta^\dagger\beta$, and therefore $[1-X\beta]\mathfrak{A}=(1-Y_1\beta^\dagger\beta)\mathfrak{A}=S$. Conversely by (A5), $1X\beta=1-S\mathfrak{A}^{-1}$ possesses a solution if and only if $(1-S\mathfrak{A}^{-1})(1-\beta^\dagger\beta)=0$, and then the solution is $X=(1-S\mathfrak{A}^{-1})\beta^\dagger+Y_2(1-\beta\beta^\dagger)$. But the condition for the existence of a solution can be viewed as an equation for $1-S\mathfrak{A}^{-1}$, and because it is homogeneous it always satisfies the condition for the existence of a solution. The solution is $1-S\mathfrak{A}^{-1}=Y_1\beta^\dagger\beta$, where I used the fact the $1-\beta^\dagger\beta$ is a hermitian idempotent and thus $(1-\beta^\dagger\beta)^\dagger=(1-\beta^\dagger\beta)$ by (A2.3). Using this result in the expression for X completes the proof.

Corollary II.2 Let M be a matrix such that βM is nonsingular. Then $S=[1-N(\beta M)^{-1}\beta]\mathfrak{A}$ possesses a solution for N if and only if S is of the form $S=(1-Y_1\beta^\dagger\beta)\mathfrak{A}$. The solution is $N=Y_1\beta^\dagger\beta M$, where Y_1 is an arbitrary $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix.

Proof: In Theorem II.1 let $X=N(\beta M)^{-1}$. Then $N=[N(\beta M)^{-1}]\beta M=[Y_1\beta^\dagger+Y_2(1-\beta\beta^\dagger)]\beta M=Y_1\beta^\dagger\beta M$.

This corollary enables us to construct an integration method with stability characteristics corresponding to any member of the collection of all matrices of the form $(1-Y_1\beta^\dagger\beta)\mathfrak{A}$. This can be done for any M and any system of differential equations but becomes a useful device only if the collection contains a member with desirable stability properties.

What about the possibility of determining not only N but also M from S? If this is to be done, then the equation for S, equation (II-57), must be augmented by another equation involving M and N. The two equations would then have to be solved simultaneously. The conclusion that $F[z(x+h), x+h]=0$ for an arbitrary linear problem if and only if $\beta(M-N)=0$ strongly suggests that we take $\beta(M-N)=0$ as the second equation. We shall need some preliminary results.

Theorem II.3 Let $S=[1-N(\beta M)^{-1}\beta]\mathfrak{A}$. Then $\beta S=0$ if and only if $\beta(M-N)=0$ if and only if $\beta N(\beta M)^{-1}=1$.

Proof: Since βM is nonsingular, we have immediately that $\beta(M-N)=0$ if and only if $\beta N(\beta M)^{-1}=1$. Since $\mathfrak{A}$ is nonsingular, it is true that $\beta S=0$ if and only if $\beta N(\beta M)^{-1}\beta=\beta$. From (A6) it follows that there always exists a solution of this equation for $\beta N(\beta M)^{-1}$, and it is given by $\beta N(\beta M)^{-1}=\beta\beta^\dagger+Y(1-\beta\beta^\dagger)$. Multiplying this result by βM on the right and using the property (A1.1) lead to $\beta N=\beta M$ and hence $\beta(M-N)=0$.

Theorem II.4 Let S be chosen as in Theorem II.1, that is, $S=(1-Y_1\beta^\dagger\beta)\mathfrak{A}$. Then $\beta S=0$ if and only if $Y_1=\beta^\dagger\beta+Y_3-\beta^\dagger\beta Y_3\beta^\dagger\beta$, where Y_3 is an arbitrary $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix. This choice for Y_1 gives $S=(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)\mathcal{A}$. Furthermore $\beta N(\beta M)^{-1}=1$ if and only if $\beta\beta^\dagger=1$ if and only if $\beta_\alpha\beta_\alpha^\dagger=1$ for $\alpha=0, 1, \ldots, m$.

Proof: Since $\beta S=(\beta-\beta Y_1\beta^\dagger\beta)\mathcal{A}$ and $\mathcal{A}$ is nonsingular, we see that $\beta S=0$ if and only if $\beta Y_1\beta^\dagger\beta=\beta$. But from (A6) we find that the condition for a solution is identically satisfied and that the solution for Y_1 is given by $Y_1=\beta^\dagger\beta+Y_3-\beta^\dagger\beta Y_3\beta^\dagger\beta$. From this it follows by direct computation that $S=(1-Y_1\beta^\dagger\beta)\mathcal{A}=(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)\mathcal{A}$. If we use the same form for Y_1 in the expression for $N(\beta M)^{-1}=X$ given in Theorem II.1, then directly $\beta N(\beta M)^{-1}=\beta\beta^\dagger+\beta Y_2(1-\beta\beta^\dagger)$ and hence $\beta N(\beta M)^{-1}=1$ if and only if $\beta Y_2(1-\beta\beta^\dagger)=(1-\beta\beta^\dagger)$. Applying (A6) to this we see that a solution for Y_2 exists if and only if $\beta\beta^\dagger=1$. But using equation (II-37) and property (A4.1) gives $\beta\beta^\dagger=\oplus\sum_{\alpha=0}^{m}\beta_\alpha\beta_\alpha^\dagger$ and therefore $\beta\beta^\dagger=1$ if and only if $\beta_\alpha\beta_\alpha^\dagger=1$.

Corollary II.5 The pair of equations $[1-N(\beta M)^{-1}\beta]\mathcal{A}=S$ and $\beta(M-N)=0$ can be solved for N and M if and only if $\beta\beta^\dagger=1$ and $S=\Delta\mathcal{A}$, where $\Delta=(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)$. The solution is $N=(1-\Delta^\dagger\Delta)Y_4$ and $M=N+(1-\beta^\dagger\beta)Y_0$. The $(m+1)(q+1)n\times(m+1)n$ matrices Y_0 and Y_4 and the $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix Y_3 are arbitrary except that Y_3 and Y_4 must be such that $\beta(1-\Delta^\dagger\Delta)Y_4$ is nonsingular.

Proof: Applying (A6) to $\beta(M-N)=0$ shows that $M=N+(1-\beta^\dagger\beta)Y_0$. The equation $\beta(M-N)=0$ also gives $S=[1-N(\beta N)^{-1}\beta]\mathcal{A}$. From Theorem II.1, with $X=N(\beta N)^{-1}$, we conclude that $N(\beta N)^{-1}=Y_1\beta^\dagger+Y_2(1-\beta\beta^\dagger)$ and $S=(1-Y_1\beta^\dagger\beta)\mathcal{A}$. By Theorem II.3 we also have that $\beta S=0$ and $\beta N(\beta M)^{-1}=1$. These facts in turn imply, by Theorem II.4, that $S=(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)\mathcal{A}$, $\beta\beta^\dagger=1$, and $N(\beta N)^{-1}=[1+(1-\beta^\dagger\beta)Y_3]\beta^\dagger$. If the last expression for $N(\beta N)^{-1}$ is multiplied by βN from the right, then it leads to $\Delta N=0$, which can always be solved for N by (A6), and the solution is $N=(1-\Delta^\dagger\Delta)Y_4$. But the requirement that βN be nonsingular imposes the condition that $\beta(1-\Delta^\dagger\Delta)Y_4$ be nonsingular. To verify that N, as given, satisfies the equation for S, we use the identity $N=(1-\Delta)N$ and from this it follows that $N(\beta N)^{-1}=(1-\Delta)[N(\beta N)^{-1}]=\{[1+(1-\beta^\dagger\beta)Y_3]\beta^\dagger\beta\}N(\beta N)^{-1}=[1+(1-\beta^\dagger\beta)Y_3]\beta^\dagger$, and this then leads to the required form for S.

This corollary, like Corollary II.2, permits us to construct an integration method with stability characteristics corresponding to any member of the collection of all matrices with the form $(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)\mathcal{A}$ when the differential equations satisfy the condition $\beta\beta^\dagger=1$. This condition will be satisfied whenever β_α is of full-row rank as would always be the case for differential equations in normal form. If β_α is of full-row rank, then β_α^* is of full-column rank and, by (A3), $\beta_\alpha^\dagger=\beta_\alpha^*(\beta_\alpha\beta_\alpha^*)^{-1}$, from which it follows that $\beta_\alpha\beta_\alpha^\dagger=(\beta_\alpha\beta_\alpha^*)(\beta_\alpha\beta_\alpha^*)^{-1}=1$. However, it is important to note that if we are given the form of N supplied by Corollary II.5, then it can be used in an integration method whether or not $\beta_\alpha\beta_\alpha^\dagger=1$. This realization when combined with Corollaries II.2 and II.5 produces the following theorem:

Theorem II.6 Let S be the stability matrix for the general (M,N)-Nordsieck integration method. The choice $N=Y_1\beta^\dagger\beta M$ implies that $S=(1-Y_1\beta^\dagger\beta)\mathcal{A}$, where Y_1 is an arbitrary $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix and M is arbitrary except that βM must be nonsingular. Let $\Delta=(1-\beta^\dagger\beta)(1-Y_3\beta^\dagger\beta)$, where Y_3 is an $(m+1)(q+1)n\times(m+1)(q+1)n$ matrix. The choices $N=(1-\Delta^\dagger\Delta)Y_4$ and $M=N+(1-\beta^\dagger\beta)Y_0$ imply $S=\Delta\mathcal{A}$, where Y_0 and Y_4 are $(m+1)(q+1)n\times(m+1)n$ matrices. The matrices Y_0, Y_3, and Y_4 are arbitrary except that Y_3 and Y_4 are constrained by the condition that $\beta(1-\Delta^\dagger\Delta)Y_4$ be nonsingular.

Proof: Simply calculate $[1-N(\beta M)^{-1}\beta]\mathcal{A}$ for the first case. For the second case observe that $\beta M=\beta N$ and $N=(1-\Delta)N=[1+(1-\beta^\dagger\beta)Y_3]\beta^\dagger\beta N$, which implies $N(\beta N)^{-1}=[1+(1-\beta^\dagger\beta)Y_3]\beta^\dagger$.

Because of this theorem we can obtain, at will, any member of a subset of the collection of all stability matrices simply by choosing either

$$N=Y_1\beta^\dagger\beta M=(1-S\mathcal{A}^{-1})M$$

or

$$N=(1-\Delta^\dagger\Delta)\,Y_4=\left[1-(S\mathcal{A}^{-1})^\dagger(S\mathcal{A}^{-1})\right]Y_4$$

The choice of S is restricted to the forms given in Theorem II.6. It is interesting to ask, Does this restricted collection of stability matrices contain the most stable case corresponding to $S=0$? That is, can $S=0$ be solved for either Y_1 or Y_3? The application of (A5) to the appropriate form of S in the equation $S=0$ shows that a solution for Y_1 or Y_3 exists if and only if $\beta^\dagger\beta=1$, and hence $S=0$ will generally not be a member because it can easily be shown that $\beta^\dagger\beta\neq 1$ for $q>0$. Since $\beta=\oplus\sum_\alpha\beta_\alpha$, it follows from (A4) that $\beta^\dagger\beta=1$ if and only if $\beta_\alpha^\dagger\beta_\alpha=1_{n(q+1)}$ for all α, and hence rank $(\beta_\alpha^\dagger\beta_\alpha)=n(q+1)$. But from (A5) we see that rank $(\beta_\alpha^\dagger\beta_\alpha)=$rank $(\beta_\alpha)\leq n$. Consequently the condition $\beta^\dagger\beta=1$ can be satisfied only for $q=0$, if then.

The stability matrix contains contributions from each of the $m+1$ points that are involved in the integration. The contribution of each point can be made independent of the other points by suitably restricting the choices for the matrices M and N. This then permits one to obtain results analogous to Theorem II.6 at each of the $m+1$ points.

Theorem II.7 Let S be the stability matrix for the general (M,N)-Nordsieck integration method and suppose (1) that $M=\oplus\sum_{\alpha=0}^{m} M_\alpha$ and $N=\oplus\sum_{\alpha=0}^{m} N_\alpha$, where M_α and N_α are $n(q+1)\times n$ matrices or (2) that $N=\oplus\sum_{\alpha=0}^{m} N_\alpha$ and $M=N+(1-\beta^\dagger\beta)\,Y_0$, where Y_0 is an arbitrary $(m+1)(q+1)n\times(m+1)n$ matrix. Then $S=\oplus\sum_{\alpha=0}^{m} S_\alpha$, where S_α is an $n(q+1)\times n(q+1)$ matrix. If condition (1) holds, then $S_\alpha=\left[1-N_\alpha(\beta_\alpha M_\alpha)^{-1}\beta_\alpha\right]A(1;q)$. Furthermore the choice $N_\alpha=Y_1\beta_\alpha^\dagger\beta_\alpha M_\alpha$ implies that $S_\alpha=(1-Y_1\beta_\alpha^\dagger\beta_\alpha)A(1;q)$ where Y_1 is an arbitrary $n(q+1)\times n(q+1)$ matrix and M_α is arbitrary except that $\beta_\alpha M_\alpha$ must be nonsingular. If condition (2) holds, then $S_\alpha=[1-N_\alpha(\beta_\alpha N_\alpha)^{-1}\beta_\alpha]A(1;q)$. Let $\Delta_\alpha=(1-\beta_\alpha^\dagger\beta_\alpha)(1-Y_3\beta_\alpha^\dagger\beta_\alpha)$, where Y_3 is an $n(q+1)\times n(q+1)$ matrix. The choice $N_\alpha=(1-\Delta_\alpha^\dagger\Delta_\alpha)\,Y_4$, where Y_4 is an $n(q+1)\times n$ matrix, implies $S_\alpha=(1-\beta_\alpha^\dagger\beta_\alpha)\,(1-Y_3\beta_\alpha^\dagger\beta_\alpha)A(1;q)$. The matrices Y_3 and Y_4 are arbitrary except that $\beta_\alpha(1-\Delta_\alpha^\dagger\Delta_\alpha)\,Y_4$ must be nonsingular.

Proof: Observe that, if condition (1) holds, then

$$(\beta M)^{-1}=\left[\left(\oplus\sum_\alpha\beta_\alpha\right)\left(\oplus\sum_\gamma M_\gamma\right)\right]^{-1}=\left[\oplus\sum_\alpha\beta_\alpha M_\alpha\right]^{-1}=\oplus\sum_\alpha(\beta_\alpha M_\alpha)^{-1}$$

Then using this we find that

$$S=\left\{\oplus\sum_{\alpha=0}^{m}1_{n(q+1)}-\left(\oplus\sum_{\alpha=0}^{m}N_\alpha\right)\left[\oplus\sum_{\gamma=0}^{m}(\beta_\gamma M_\gamma)^{-1}\right]\left(\oplus\sum_{\delta=0}^{m}\beta_\delta\right)\right\}\left[\oplus\sum_{\lambda=0}^{m}A(1;q)\right]$$

$$=\left\{\oplus\sum_{\alpha=0}^{m}\left[1_{n(q+1)}-N_\alpha(\beta_\alpha M_\alpha)^{-1}\beta_\alpha\right|\right\}\left[\oplus\sum_{\lambda=0}^{m}A(1;q)\right]$$

$$=\oplus\sum_{\alpha=0}^{m}\left|1_{n(q+1)}-N_\alpha(\beta_\alpha M_\alpha)^{-1}\beta_\alpha\right|A(1;q)$$

$$=\oplus\sum_{\alpha=0}^{m}S_\alpha$$

If condition (2) holds, then $\beta M = \beta N$, and proceeding as above establishes the result that $S = \oplus \sum_{\alpha=0}^{m} S_\alpha$. The balance of the theorem follows by direct computation of S_α as done in Theorem II.6 for S itself.

If M is chosen as in Theorem II.7(1), then the $m+1$ points are decoupled with respect to the determination of z_{q+1}. However, choosing M as in Theorem II.7(2) does not necessarily lead to such a decoupling because of the arbitrariness of Y_0.

Some Special Cases

I shall confine my attention to the forms of N and M of Theorem II.7(1), which lead to a decoupling of points and reduce the problem to the case $m=0$ (one-step method) for which $\beta = \beta_0$. Obviously one could look at special cases by considering particular differential equations and tailoring the methods for these equations. But one can also look at special cases by examining the behavior of the method in the limits of small and large step size. Intuitively one expects to find results of broader applicability by looking at the limiting behavior as $h \to 0$ and $h \to \infty$. In particular, I shall examine the limiting stability behavior and obtain results which are exact in the limit.

Suppose we define $\tilde{\beta}_\alpha$ as

$$\tilde{\beta}_\alpha \equiv \frac{\partial f(\xi,\, x+h-\alpha h)}{\partial \xi}\bigg|_{\xi = H^{-1} w_\alpha} = \beta_\alpha H \tag{II-58}$$

and assume that the limits

$$\lim_{h \to 0} \tilde{\beta}_\alpha = \tilde{\beta}_\alpha(0) = \left[\tilde{\beta}_{\alpha 0}(0), \ldots, \tilde{\beta}_{\alpha q}(0)\right] \tag{II-59}$$

$$\lim_{h \to \infty} \tilde{\beta}_\alpha = \tilde{\beta}_\alpha(\infty) = \left[\tilde{\beta}_{\alpha 0}(\infty), \ldots, \tilde{\beta}_{\alpha q}(\infty)\right] \tag{II-60}$$

exist. Then, since $\beta_\alpha = \tilde{\beta}_\alpha H^{-1}$, for a p^{th} order differential equation ($p \le q$) we have

$$\beta_\alpha = \begin{cases} e_0^* \otimes \left[0!\, h^{-0} \tilde{\beta}_{\alpha 0}(\infty)\right] & \text{as } h \to \infty \\[2ex] e_p^* \otimes \left[p!\, h^{-p} \tilde{\beta}_{\alpha p}(0)\right] & \text{as } h \to 0 \end{cases} \tag{II-61}$$

as the limiting behavior. The vector e_k, $k = 0, 1, \ldots, q$, is a $(q+1)$-dimensional vector whose k^{th} component is unity and all other components are zero. Note that in equation (II-61) the order of the differential equation is immaterial in the limit $h \to \infty$. The limiting behavior in equation (II-61) suggests that we explore the $m=0$ case for stability associated with the form

$$\beta = \beta_0 = b^* \otimes Z \tag{II-62}$$

where b is a $(q+1)$-dimensional vector and Z is an $n \times n$ nonsingular matrix. By (A4.2), (A2.2), (A2.1), and (A3) it follows that

$$\beta^\dagger = (b^* b)^{-1} b \otimes Z^{-1} \tag{II-63}$$

and from this we obtain

$$\beta^{\dagger}\beta = (b^*b)^{-1}bb^*\otimes 1_n \tag{II-64}$$

Suppose we also restrict Y_1 of Theorem II.7 to the form

$$Y_1 = -\epsilon L\otimes 1_n \tag{II-65}$$

where ϵ is a complex number and L is a $(q+1)\times(q+1)$ matrix. Then this leads to

$$S = \left(1 - Y_1\beta^{\dagger}\beta\right)A(1;q) = \left\{\left[1_{q+1} + \epsilon(b^*b)^{-1}Lbb^*\right]P(1;q)\right\}\otimes 1_n \tag{II-66}$$

It is known that the Pascal matrix $P(1,\ q)$ has the Jordan canonical form $1_{q+1} + J_{q+1}$. That is, there exists a nonsingular matrix T such that

$$T^{-1}P(1;q)T = 1_{q+1} + J_{q+1} \tag{II-67}$$

and hence

$$S' \equiv \left(T^{-1}\otimes 1_n\right)S_{\alpha}\left(T\otimes 1_n\right) = \left(J_{q+1} + 1_{q+1} + \epsilon ut^*\right)\otimes 1_n \equiv U\otimes 1_n \tag{II-68}$$

where

$$u \equiv (b^*b)^{-1}T^{-1}Lb \tag{II-69}$$

$$t^* \equiv b^*PT \tag{II-70}$$

The eigenvalues of S are the eigenvalues of S', and these can be altered only by making changes in the vector u and the number ϵ because the vector t is presumed known. If λ is an eigenvalue of S and $\mu = \lambda - 1$, then the characteristic equation for S' is

$$|S' - \lambda 1| = \left|U - \lambda 1_{q+1}\right|^n = \left|J_{q+1} + \epsilon ut^* - \mu 1_{q+1}\right|^n = 0 \tag{II-71}$$

which determines the values μ_i, $i = 0,\ 1,\ \ldots,\ q$ for a given u. Conversely it should be possible to prescribe the $q+1$ eigenvalues μ_i and use these to determine the $q+1$ components of u. But if we know u, then the defining equation for u, equation (II-69), can be solved for L by using (A6) and (A3) to get

$$L = Tub^* + Y'\left[1_{q+1} - (b^*b)^{-1}bb^*\right] \tag{II-72}$$

where Y' is an arbitrary $(q+1)\times(q+1)$ matrix. The combination of Theorem II.7 (1) for $m = 0$ and equations (II-64), (II-65), and (II-72) shows that

$$\begin{aligned} N &= -\epsilon\left[(Tub^*)\otimes 1_n\right]M \\ \beta N &= -\epsilon\left(\frac{b^*Lb}{b^*b}\right)\beta M = -\epsilon(b^*Tu)\beta M \end{aligned} \tag{II-73}$$

The second member of equation (II-73) leads to the conclusion that

$$\beta(N - M) = 0 \text{ if and only if } \epsilon = -\left(\frac{b^*b}{b^*Lb}\right) = -(b^*Tu)^{-1} \tag{II-74}$$

We must now try to find a computationally convenient connection between the vector u and eigenvalues μ_i. If $adj(A)$ is the adjugate matrix (sometimes called the adjoint matrix) of any matrix A, then it can be shown that

$$|A+ut^*|=|A|+t^*[adj(A)]u \tag{II-75}$$

The elements of $adj(A)$ are the cofactors of the elements of A. Furthermore it can be shown that

$$adj(J_{q+1}-\lambda 1_{q+1})=\sum_{l=1}^{q+1}(-\lambda)^{q+1-l}(-J_{q+1})^{l-1}=\sum_{k=0}^{q}(-\lambda)^{q-k}(-J_{q+1})^k \tag{II-76}$$

$$|J_{q+1}-\lambda 1_{q+1}|=(-\lambda)^{q+1} \tag{II-77}$$

An expression for the determinant in equation (II-71) can be obtained by combining equations (II-75) to (II-77).

$$(-1)^{q+1}|J_{q+1}-\mu 1_{q+1}+\epsilon ut^*|=\mu^{q+1}-\epsilon\sum_{k=0}^{q}\mu^{q-k}(t^*J_{q+1}^k u) \tag{II-78}$$

If μ_i, $i=0, 1, \ldots, q$, are the roots of this polynomial, then the elementary symmetric functions of these roots are defined by

$$\mathrm{S}_l(\mu_i)=\sum_{0\le i_1<i_2<\ldots<i_l\le q}\mu_{i_1}\mu_{i_2}\cdots\mu_{i_l} \qquad l=1, 2, \ldots, q+1 \tag{II-79}$$

But the polynomial (II-78) can also be written in terms of its roots.

$$\prod_{i=0}^{q}(\mu-\mu_i)=\mu^{q+1}-\sum_{k=0}^{q}\mu^{q-k}(-1)^k\mathrm{S}_{k+1} \tag{II-80}$$

A comparison of equations (II-78) and (II-80) shows that

$$\epsilon t^*J_{q+1}^k u=(-1)^k\mathrm{S}_{k+1}(\mu_i) \qquad k=0, 1, \ldots, q \tag{II-81}$$

and this system of equations can be viewed as a set of linear equations for u, giving u as a function of ϵ, t, and the roots μ_i. This system of equations can be written more compactly as

$$\epsilon\Gamma u=c \tag{II-82}$$

where c is the vector

$$c^*\equiv[(-1)^0\mathrm{S}_1^*, (-1)^1\mathrm{S}_2^*, \ldots, (-1)^q\mathrm{S}_{q+1}^*]=(c_0^*, c_1^*, \ldots, c_q^*) \tag{II-83}$$

and the matrix Γ is

$$\Gamma^*=(\gamma_0, \gamma_1, \ldots, \gamma_q) \tag{II-84}$$

The vectors γ_k can be conveniently expressed by using the representation

$$J_{q+1}^k=\sum_{i=0}^{q-k}e_ie_{i+k}^*$$

to obtain the result

$$\gamma_k^* \equiv t^* J_{q+1}^k = \sum_{i=0}^{q-k} \left(t^* e_i\right) e_{i+k}^* \tag{II-85}$$

Thus Γ has the upper triangular form

$$\Gamma = \begin{bmatrix} t^*e_0 & t^*e_1 & t^*e_2 & \cdots & t^*e_q \\ 0 & t^*e_0 & t^*e_1 & \cdots & t^*e_{q-1} \\ 0 & 0 & t^*e_0 & \cdots & t^*e_{q-2} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & \cdots & t^*e_0 \end{bmatrix} = \sum_{k=0}^{q} \left(t^*e_k\right) J_{q+1}^k.$$

We shall now examine the solutions of equation (II-82) for the vector $u(\epsilon)$. Clearly the determinant of the matrix Γ is $|\Gamma| = (t^*e_0)^{q+1}$, and so Γ is singular if and only if the zero component of t vanishes. But then equation (II-82) and the form of Γ imply that the zero component of u is arbitrary and also that $S_{q+1}=0$. The latter then in turn implies that $\mu_q=0$, and hence $\lambda_q=1$. More generally, it follows from the structure of Γ that rank $\Gamma=q+1-j$ if and only if for some j, $0 \le j \le q+1$, $t^*e_j \neq 0$ and $t^*e_k=0$ for all k such that $0 \le k < j$ if and only if

$$\Gamma = \begin{bmatrix} 0 & \Gamma_{12} \\ 0 & 0 \end{bmatrix}$$

$$\Gamma^\dagger = \begin{bmatrix} 0 & 0 \\ \Gamma_{12}^{-1} & 0 \end{bmatrix}$$

where 0 is a zero matrix and Γ_{12} is the upper triangular, nonsingular $(q+1-j)\times(q+1-j)$ submatrix of Γ for $j<q+1$. If $j=q+1$, then Γ is the zero matrix. Using the form of Γ and $\Gamma^\dagger$, it follows that

$$\Gamma\Gamma^\dagger = 1_{q+1-j} \oplus 0_j$$

$$\Gamma^\dagger\Gamma = 0_j \oplus 1_{q+1-j}$$

$$1_{q+1} - \Gamma^\dagger\Gamma = 1_j \oplus 0_{q+1-j}$$

Utilizing this information, together with (A6), we conclude that when rank $\Gamma = q+1-j$ then equation (II-82) has the solution

$$u(\epsilon) = \epsilon^{-1}\Gamma^\dagger c + (1_j \oplus 0_{q+1-j})y \tag{II-86}$$

if and only if $(1_{q+1-j} \oplus 0_j)c = c$, where y is an arbitrary vector. If we evaluate $u(\epsilon)$ at ϵ_0 and eliminate $\Gamma^\dagger c$ between the two equations, we find

$$u(\epsilon) = \epsilon^{-1}\epsilon_0 u(\epsilon_0) + (1 - \epsilon^{-1}\epsilon_0)(1_j \oplus 0_{q+1-j})y \tag{II-87}$$

The form of the solution given in equation (II-86) shows that c can only affect the last $(q+1-j)$ components of $u(\epsilon)$ and that the arbitrary y can only affect the first j components of $u(\epsilon)$. The condition for the existence of the solution (II-86) can be satisfied if and only if the last j components of c vanish; that is, if and only if $s_{q+2-k}=0$, if and only if $\mu_{q+1-k}=0$, if and only if $\lambda_{q+1-k}=1$ for all k such that $1 \le k \le j$.

Suppose u is as given in equation (II-86). Then

$$\epsilon b^* T u = b^* T \Gamma^\dagger c + \epsilon b^* T(1_j \oplus 0_{q+1-j}) y$$

If $b^* T \Gamma^\dagger c = -1$, then $b^* T u = -\epsilon^{-1}$ if and only if $b^* T(1_j \oplus 0_{q+1-j}) y = 0$, which can always be satisfied by $y=0$. If $b^* T \Gamma^\dagger c \neq -1$ and $b^* T(1_j \oplus 0_{q+1-j}) y \neq 0$, then $b^* T u = -\epsilon^{-1}$ if and only if

$$\epsilon = \frac{-(1 + b^* T \Gamma^\dagger c)}{b^* T(1_j \oplus 0_{q+1-j}) y} \tag{II-88}$$

Hence, using equation (II-74), it follows that the arbitrariness of y permits us to achieve $\beta(N-M)=0$ in these two situations. The condition $b^* T(1_j \oplus 0_{q+1-j}) y \neq 0$ implies that $j>0$. If $j=0$, then $\Gamma^\dagger = \Gamma^{-1}$ and then $b^* T u = -\epsilon^{-1}$ if and only if $b^* T \Gamma^{-1} c = -1$. From the foregoing we see that satisfying the condition $b^* T u = -\epsilon^{-1}$ presents no difficulty except perhaps when Γ is of rank $q+1$. In this situation $b^* T(1_j \oplus 0_{q+1-j}) y \equiv 0$ because $j=0$, and so the vectors b and c are constrained by $b^* T \Gamma^{-1} c = -1$ because $\Gamma^\dagger = \Gamma^{-1}$. Now we might fortuitously select a pair of vectors b and c which do satisfy $b^* T \Gamma^{-1} c = -1$. But, more generally, we must expect that independently selected vectors b and c will not satisfy the constraint. If we choose to prescribe the stability characteristics, as determined by the vector c, then we must be content to achieve this stability for a limited class of differential equations characterized by β as given in equation (II-62). Conversely, if we wish to allow complete freedom in b, then this restricts the kind of stability that can be obtained. The constraint $b^* T \Gamma^{-1} c = -1$ is linear in c and nonlinear in b because Γ itself is dependent on b. The linearity in c permits us to solve the constraint for c in terms of b. The use of (A6) and (A3) shows that $b^* T \Gamma^{-1} c = -1$ can always be solved for c and that the solution is

$$c(y) = -(x^* x)^{-1} x + \left[1_{q+1} - (x^* x)^{-1} x x^*\right] y$$

where y is an arbitrary $(q+1)$-dimensional vector and $x^* = b^* T \Gamma^{-1}$. By comparing equations (II-80) and (II-83) we see that the stability characteristics are governed by the roots of

$$\mu^{q+1} - \sum_{k=0}^{q} c_k(y) \mu^{q-k} = 0$$

and so, if we use y as a set of $(q+1)$ parameters, then we can find the optimally stable method for a given vector b. The results of this section are summarized by the next theorem.

Theorem III.1 Suppose that Theorem II.7(1) holds and that $m=0$. Furthermore let

(1) $N = Y_1 \beta^\dagger \beta M$
(2) $Y_1 = -\epsilon L \otimes 1_n$
(3) $\beta = b^* \otimes Z$

where ϵ is a complex number, L is a $(q+1) \times (q+1)$ matrix, b is a $(q+1)$-dimensional vector, and Z is an $n \times n$ nonsingular matrix. Then

(4) $\beta(N-M) = 0$ if and only if $\epsilon = -(b^* b / b^* L b) = -(b^* T u)^{-1}$.

(5) The stability matrix S is given by $S = [T(J_{q+1} + 1_{q+1} + \epsilon u t^*) T^{-1}] \otimes 1_n$, where T is a nonsingular $(q+1) \times (q+1)$ matrix which reduces the Pascal matrix $P(1;q)$ to Jordan canonical form, $T^{-1} P(1;q) T = 1_{q+1} + J_{q+1}$, and where $u = (b^* b)^{-1} T^{-1} L b$, $t^* = b^* P T$.

(6) $N = -\epsilon[(T u b^*) \otimes 1_n] M$.

(7) Every eigenvalue λ of S is a root of the polynomial $\mu^{q+1} - \epsilon \sum_{k=0}^{q} \mu^{q-k} \left(t^* J_{q+1}^k u\right)$ of degree $q+1$, where $\mu = \lambda - 1$. If λ is one of the roots of this polynomial with multiplicity m, then λ is an eigenvalue of S with multiplicity nm.

(8) The vector u can be regarded as a solution of the system of linear equations $\epsilon\Gamma u = c$, where Γ is the $(q+1)\times(q+1)$ matrix $\Gamma^* = (\gamma_0, \gamma_1, \ldots, \gamma_q)$. The $(q+1)$-dimensional vectors γ_k are given by

$$\gamma_k^* = t^* J_{q+1}^k = \sum_{i=0}^{q-k} (t^* e_i) e_{i+k}^* \qquad k = 0, 1, \ldots, q$$

and the vector c is given by $c^* = [(-1)^0 \mathcal{S}_1^*, (-1)^1 \mathcal{S}_2^*, \ldots, (-1)^q \mathcal{S}_{q+1}^*]$, where $\mathcal{S}_l$ are the elementary symmetric functions and are defined by

$$\mathcal{S}_l(\mu_i) = \sum_{0 \le i_1 < i_2 \ldots < i_l \le q} \mu_{i_1} \mu_{i_2} \cdots \mu_{i_l} \qquad l = 1, 2, \ldots, q+1$$

(9) The matrix Γ is upper triangular and is of rank $q+1-j$ if and only if for some integer j, $0 \le j \le q+1$, $t^* e_j \ne 0$ and $t^* e_k = 0$ for all k such that $0 \le k < j$.

(10) If Γ is of rank $q+1-j$, then the eigenvalues λ_k of S are arbitrary for $0 \le k \le q-j$ and equal to unity for all k such that $q+1-j \le k \le q$. A solution of $\epsilon\Gamma u = c$ for u exists if and only if $(1_{q+1-j} \oplus 0_j)c = c$, and the most general solution is $u = \epsilon^{-1}\Gamma^\dagger c + (1_j \oplus 0_{q+1-j})y$, where y is an arbitrary $(q+1)$-dimensional vector. The solution can also be written in the form $u(\epsilon) = \epsilon^{-1}\epsilon_0 u(\epsilon_0) + (1 - \epsilon^{-1}\epsilon_0)(1_j \oplus 0_{q+1-j})y$.

(11) There exists an ϵ such that $b^* T u = -\epsilon^{-1}$ if and only if either $b^* T \Gamma^\dagger c = -1$ and $b^* T(1_j \oplus 0_{q+1-j})y = 0$ or $b^* T\Gamma^\dagger c \ne -1$ and $b^* T(1_j \oplus 0_{q+1-j})y \ne 0$.

(12) Suppose Γ is of rank $q+1$. Then $b^* T \Gamma^\dagger c = b^* T \Gamma^{-1} c = -1$ if and only if $c(y) = -(x^* x)^{-1} x + [1_{q+1} - (x^* x)^{-1} x x^*]y$, where $x^* = b^* T \Gamma^{-1}$ and y is an arbitrary $(q+1)$-dimensional vector. For this choice of the vector c the eigenvalues $\lambda_k(y)$ of S are the roots of the polynomial

$$\mu^{q+1} - \sum_{k=0}^{q} c_k(y) \mu^{q-k}$$

where $\mu = \lambda - 1$.

The foregoing theorem deals exclusively with properties associated with special cases of the general integration methods of Definition I.2. I wish to specialize these results even more by making a commitment to a form for M in Theorem III.1(6). Suppose we try $M = \ell \otimes V$, where ℓ is a $(q+1)$-dimensional vector and V is an $n \times n$ matrix. Then this implies that $N = -\epsilon b^* \ell (Tu \otimes V)$. Can we now find an ϵ and an ℓ such that $N = \nu(\ell \otimes V) = \nu M$ for some complex number ν? This will be true if and only if $\nu\ell = -\epsilon b^* \ell T u$. If this equation is multiplied by b^*, we find that this requires $\nu = -\epsilon(b^* T u)$, and with this choice for ν we see that ℓ must be a solution of the homogeneous equations

$$\left(1_{q+1} - \frac{Tub^*}{b^* Tu}\right)\ell = 0 \tag{II-89}$$

Nontrivial solutions for ℓ will exist if and only if the determinant $|1_{q+1} - (b^* Tu)^{-1} Tub|$ vanishes. But from equation (II-75)

$$\begin{aligned} |1_{q+1} - (b^* Tu)^{-1} Tub^*| &= |1_{q+1}| - (b^* Tu)^{-1} b^* [adj(1_{q+1})] Tu \\ &= 1 - (b^* Tu)^{-1} b^* Tu \\ &\equiv 0 \end{aligned}$$

Hence we are guaranteed that nontrivial solutions will always exist for equation (II-89), and one can easily verify that, for any complex number α, $\ell = \alpha T u$ is a solution. The requirement that $(\beta M)^{-1}$ exist leads to the condition that V be nonsingular.

Theorem III.2 In Theorem III.1(6) choose $M = \ell \otimes V$, where ℓ is a $(q+1)$-dimensional vector and V is an $n \times n$ nonsingular matrix. If ν is a complex number such that $\nu = -\epsilon(b^* Tu)$, then any ℓ which satisfies the homogeneous equations $[1_{q+1} - (b^* Tu)^{-1} Tub^*]\ell = 0$ will yield $N = \nu M$ for arbitrary V. In particular, the vector $\ell = \alpha Tu$ is such a solution for an arbitrary complex number α.

We shall soon see that the integration methods of Theorem III.2 contain the Gear and Nordsieck methods of integration as special cases.

The limiting forms of β_α given in equation (II-61) suggest that we calculate the vectors t, u, and $-Tu$ of Theorem III.1 for $b = e_k$, $0 \leq k \leq q$, because for these limiting cases the three vectors are independent of the form of the differential equations and in the limit $h \to \infty$ they are also independent of their order. The results of the calculation for $k = 0, 1, \ldots, 8$ and $q = k, k+1, \ldots, 8$ subject to the condition that $q > 0$ are shown in table I. An examination of this table discloses that in all cases $-b^* Tu = 1$. Hence, the choice $\epsilon = 1$ satisfies Theorem III.1(4), and thus $\nu = 1$ and $N = M$ from Theorem III.2. The coefficients for Gear's method (ref. 7) and those for Nordsieck's method (refs. 2, 3, and 5) are shown in table II. A detailed comparison of the two tables shows that the Gear coefficients given in table II(a), for any given value of q, are scalar multiples of the vector $(-Tu)$ of table I for $k = 0$ and the same value of q. It should now be clear that Gear's integration method (ref. 9) can be regarded as a special case of the more general integration methods of Theorem III.2 and obtained from them by (1) choosing a one-step method ($m = 0$), (2) applying it to a first order system of equations in normal form, (3) selecting $V = 1_n$ and $\alpha^{-1} = e_1^* Tu$, and (4) solving the equations by a modified Newton iteration with no step-size control during the iteration. Note, however, that my derivation of this result shows that Gear's method is applicable to higher order differential equations as well as first order equations. This is because the $h \to \infty$ limit is independent of order as is shown in equation (II-61).

Similarly, for a p^{th} order system of differential equations ($p \geq 1$), the Nordsieck coefficients given in table II(b) for a method of polynomial degree q are related to the vector $(-Tu)$ of table I for the same value of q and $k = p$. The last $q + 1 - p$ Nordsieck coefficients of table II(b) agree with the last $q + 1 - p$ components of $(-p^{-1} Tu)$. But since the first p components of Tu are arbitrary by Theorem III.1(10), insofar as stability is concerned, the agreement could be made complete. We thus see that the Nordsieck method is also a special case of the methods of Theorem III.2 for it is (1) a one-step method ($m = 0$), (2) applied to a p^{th} order system of differential equations in normal form, and (3) obtained by choosing $V = 1_n$ and either $\alpha = 1$ (for Gear's extension, ref. 3) or $\alpha = p^{-1}$ (for LaBudde's extension, ref. 5). Gear's implementation of the Nordsieck method (ref. 9) for $p = 1$ solves the equations by the successive-substitutions iteration with no step-size control during the iteration. It is apparent that the Gear and Nordsieck methods are two aspects of the same more general method. The former represents maximum stability in the limit $h \to \infty$; the latter represents maximum stability in the limit $h \to 0$.

I still wish to consider the specialization of the parameter α and those components of ℓ not determined by stability considerations in the $h \to 0$ limit. My analysis will lead to vectors ℓ which differ from those of Nordsieck, Gear, and LaBudde. Consider a polynomial of degree R

$$y(x) = \sum_{n=0}^{R} \frac{g_n x^n}{n!} \tag{II-90}$$

where the vectors g_n are independent of x, and a p^{th}-order differential equation of the type (II-42)

$$D_p y^{(p)} + g(x) = 0 \tag{II-91}$$

where D_p is nonsingular and also independent of x. Then since

$$y^{(p)}(x) = \sum_{i=0}^{R-p} \frac{g_{i+p} x^i}{i!}$$

the differential equation will have the polynomial $y(x)$ as a solution if and only if

$$g(x) = -D_p \sum_{i=0}^{R-p} \frac{g_{i+p}x^i}{i!} \tag{II-92}$$

If we use the binomial theorem and interchange the orders of summation, we have

$$y(x+h) = \sum_{n=0}^{R} \frac{g_n(x+h)^n}{n!} = \sum_{n=0}^{R} \frac{g_n}{n!} \sum_{k=0}^{n} \binom{n}{k} h^k x^{n-k} = \sum_{k=0}^{R} \frac{h^k}{k!} \sum_{n=k}^{R} \frac{g_n x^{n-k}}{(n-k)!}$$

$$= \sum_{k=0}^{R} \frac{h^k}{k!} \sum_{i=0}^{R-k} \frac{g_{i+k}x^i}{i!} = \sum_{k=0}^{R} \frac{h^k y^{(k)}(x)}{k!}$$

which is an exact result. Since $y^{(s)}(x)$ is also a polynomial, we can replace y by $y^{(s)}$ above to obtain

$$y^{(s)}(x+h) = \sum_{k=0}^{R} \frac{h^k y^{(k+s)}(x)}{k!} = \sum_{k=0}^{R-s} \frac{h^k y^{(k+s)}(x)}{k!} = \sum_{i=s}^{R} \frac{h^{(i-s)} y^{(i)}(x)}{(i-s)}$$

where I used $y^{(k)}(x) = 0$ for $k > R$. From this it follows immediately that

$$\frac{h^s y^{(s)}(x+h)}{s!} = \sum_{i=s}^{R} \frac{\binom{i}{s} h^i y^{(i)}(x)}{i!} \tag{II-93}$$

Consequently it follows that in this case (II-8) becomes

$$\eta(x+h,\ h,\ q) = A(1;q)\eta(x,\ h,\ q) + \sigma(1,\ q,\ x) \tag{II-94}$$

where the components of σ are the remainders

$$r_s(1,\ q,\ x) = \sum_{i=q+1}^{R} \frac{\binom{i}{s} h^i y^{(i)}(x)}{i!} \tag{II-95}$$

and where $q < R$. But we can also calculate $z(x+h)$ from equation (II-51) for $m=0$ and $N = M = \ell \otimes V$ and the differential equation defined by equations (II-91) and (II-92) with $z(x) = \eta(x,\ h,\ g)$. The result is

$$z(x+h) = A(1;q)\eta(x,\ h,\ q) + \ell_p^{-1}\left(\ell e_p^{*} \otimes V\right)\sigma \tag{II-96}$$

where I used

$$\frac{h^p D_p^{-1} g(x+h)}{p!} = \frac{-h^p y^{(p)}(x+h)}{p!}$$

which is a consequence of equation (II-91) and

$$\frac{h^p y^p(x)}{p!} = \left(e_p^{*} \otimes 1_n\right)\eta(x+h,\ h,\ q)$$

in which $\eta(x+h,\ h,\ q)$ was eliminated with equation (II-94).

From equation (II-96) we see that for this special case of a p^{th} order differential equation it is the vector ℓ weighted by its p^{th} component ℓ_p which characterizes the integration, and this in turn suggests that ℓ be chosen so that $\ell_p = 1$ for simplicity. From the form of ℓ given in Theorem III.2 we find that

$$\ell_p = e_p^* \ell = 1 \text{ if and only if } \alpha^{-1} = e_p^* T u \tag{II-97}$$

which corresponds to the weighting used by Nordsieck and Gear. A comparison of $z(x+h)$ with equation (II-94) suggests that those components of ℓ which do not affect stability be chosen so as to improve the agreement between $z(x+h)$ and $\eta(x+h,\ h,\ q)$. Since $(\ell e_p^* \otimes V)\sigma = \ell \otimes (V r_p)$, we want to look at $\sigma - \ell \otimes (V r_p)$, which, for the i^{th} remainder, takes the form

$$r_i - \ell_p^{-1} \ell_i V r_p = \sum_{j=q+1}^{R} \left[\binom{j}{i} 1_n - \binom{j}{p} \ell_p^{-1} \ell_i V \right] \frac{h^j y^{(j)}(x)}{j!} \qquad i = 0, 1, 2, \ldots, q$$

where I used equation (II-95) to eliminate the remainders. Thus if we make the choice

$$\ell_i = \frac{\binom{q+1}{i} \ell_p}{\binom{q+1}{p}} = \frac{p!\,\ell_p}{i!\,(q-p+2)(q-p+3)\ldots(q+1-i)} \qquad i = 0, 1, \ldots, p-1$$

$$V = 1_n \tag{II-98}$$

for the methods of theorem III.2 in the $h \to 0$ limit, then $z(x+h)$ and $\eta(x+h,\ h,\ q)$ will agree to order $q+1$ for the subvectors $i = 0, 1, \ldots, p$ and to order q for the subvectors $i = p+1, \ldots, q$.

Can a method of the type considered in theorem III.2 be constructed for intermediate values of h but which has the appropriate limiting behavior? The answer is yes for we can easily construct the vector $\ell(h) = \ell(0) \exp(-|h/h_0|) + \ell(\infty)[1 - \exp(-|h/h_0|)]$, where h_0 is a real number which can be regarded as a parameter of the integration method. If $\ell(\infty)$ and $\ell(0)$ are the vectors for the $h \to \infty$ and $h \to 0$ limits, then $M = N = \ell(h) \otimes 1_n$ would produce such a method. Alternatively we can try to construct a vector b with the limiting behavior $\lim_{h \to \infty} b = e_0$ and $\lim_{h \to 0} b = e_p$. Of course, such a vector could be formed in a number of ways; for example, $b = e_p \exp(-|h/h_0|) + e_0[1 - \exp(-|h/h_0|)]$ is one such vector. An alternative choice might be some vector which incorporated properties of the solution $y(x)$. Let $G(k)$ be hermitian, nonnegative, semi-definite matrices for $k = 0, 1, \ldots, q$ independent of h and satisfying the conditions that $y^{(k)*} G(k) y^{(k)}$ is not zero for $k = q_1$, q_2 and is zero for $k < q_1$ and $k > q_2$, where $0 \le q_1 \le q_2 \le q$. Then we can define real numbers ϕ_k by

$$\phi_k \equiv \left(\frac{h^k}{k!} \right)^2 \frac{y^{(k)*} G(k) y^{(k)}}{\sum_{i=0}^{q} (h^i/i!)^2 y^{(i)*} G(i) y^{(i)}} \qquad k = 0, 1, 2, \ldots, q$$

Since ϕ_k can be written as

$$\phi_k = \left(\frac{h^{k-q_1} q_1!}{k!} \right)^2 \frac{y^{(k)*} G(k) y^{(k)}}{\sum_{i=0}^{q} \left(h^{i-q_1} q_1!/i! \right)^2 y^{(i)*} G(i) y^{(i)}}$$

$$= \left(\frac{h^{k-q_2} q_2!}{k!} \right)^2 \frac{y^{(k)} G(k) y^{(k)}}{\sum_{i=0}^{q} \left(h^{i-q_2} q_2!/i! \right)^2 y^{(i)*} G(i) y^{(i)}}$$

we see that

$$\lim_{h \to 0} \phi_k = \begin{cases} 1 & k = q_1 \\ 0 & k \neq q_1 \end{cases}$$

$$\lim_{h \to \infty} \phi_k = \begin{cases} 1 & k = q_2 \\ 0 & k \neq q_2 \end{cases}$$

If we choose

$$b = \sum_{k=0}^{q_2 - q_1} \phi_{k+q_1} e_{q_2 - k}$$

then $b \to e_{q_2}$ as $h \to 0$ and $b \to e_{q_1}$ as $h \to \infty$. Naturally if this choice were made for b, then in the actual calculation of ϕ_k the quantity $h^k y^{(k)}/k!$ would be replaced by $a_k(x - \alpha h)$. Whether this choice, or any other choice, for b leads to an improved integration method can only be decided on the basis of numerical computations. This aspect of the problem will not be considered here.

The choice of a vector b might lead to a violation of the condition $b^* T u = -\epsilon^{-1}$ of Theorems III.1(4) and III.2. This can only occur if Γ is of rank $q+1$ since by Theorem III.1(11) the condition can always be satisfied if Γ is singular. It can easily be shown that $t^* e_0 = b^* T e_0$, and since T is upper triangular, $b^* T e_0 = T_{00} b^* e_0$. Hence $t^* e_0 \neq 0$ if and only if $b^* e_0 \neq 0$, and so by Theorem III.1(9) Γ is nonsingular or of rank $q+1$ if and only if $b^* e_0 \neq 0$. Thus the unpleasantness associated with the computations of Theorem III.1(12) can always be avoided when

$$b = \sum_{k=0}^{q_2 - q_1} \phi_{k+q_1} e_{q_2 - k}$$

merely by assuring that $q_1 > 0$.

Step-Size and Order Changes

The discussions on the previous pages were confined to methods with a fixed integration step size h and a fixed order q. In practice, however, we might wish to alter both the order and the step size during the integration in a manner designed to give optimal results. To make these choices in a rational way, we must be able to estimate the effect of such changes on the integration error in $z(x+h)$ or, more simply, the integration error in its first n components, $y(x+h)$. If one can estimate the integration errors for methods of order $q-1$, q, and $q+1$ and also estimate their dependence on step size, then for the next step one can choose the order and step size so as to maintain the error at a given level. Let the n-dimensional vector $I_q(x+h, h)$ be the contribution to the integration error in y at $x+h$ from a step of size h with an integration method of order q. Instead of monitoring the vector I_q one could introduce a suitable norm and monitor the length of I_q, $\|I_q\|$. Clearly this is not as stringent as monitoring I_q itself, but it will generally be computationally simpler. Such a procedure was used both by Gear (ref. 8) and Hindmarsh (ref. 10), who used the truncation error as an estimate for the integration error. Unfortunately one has no way of knowing the integration error. The best one can do is to assume that it is proportional to the truncation error, designated as $T_q(x+h, h)$, which can be estimated with the first n components of $N z_{q+1}$. Suppose the step from x to $x+h$ is by a method of order q and the step from $x - \tilde{h}$ to x is by a method of order $\tilde{q}$. Then I choose to write the integration error at $x+h$ for a method of order $\bar{q}$ and step size h' as

$$I_{\bar{q}}(x+h, h') = \gamma_{\bar{q}}^{-(\bar{q}+1)} \frac{\|T_q(x+h, h)\|}{\|T_{\tilde{q}}(x, \tilde{h})\|} T_{\bar{q}}(x+h, h') \qquad \text{(II-99)}$$

where $\bar{q}$ takes the values $q-1$, q, and $q+1$. The factor $||T_q(x+h,\ h)||/||T_{\bar{q}}(x,\ \tilde{h})||$ reflects the reasonable assumption that, if the truncation error in successive steps is increasing, then the integration error will be larger than if the truncation error were decreasing. The constants $\gamma_{\bar{q}}$ are to be chosen empirically. Since only T_q is available at $x+h$, T_{q+1} and T_{q-1} must be estimated from it. Comparing methods of order $q-1$, q, and $q+1$ gives a relationship among the three truncation errors.

$$T_{q-1}(x+h,\ h)=T_q(x+h,\ h)+\frac{h^q y^{(q)}(x)}{q!}$$

$$T_{q+1}(x+h,\ h)=T_q(x+h,\ h)-\frac{h^{q+1}y^{(q+1)}(x)}{(q+1)!} \tag{II-100}$$

The same relationships can also be obtained from equation (II-4) using $s=0$ and identifying $r_0(1,\ q,\ x)$ with T_q. The truncation error for any q can also be expressed by means of the Lagrangian form of the remainder in the Taylor formula

$$T_q(x+h,\ h)=\frac{h^{q+1}y^{(q+1)}(\xi)}{(q+1)!} \qquad x<\xi<x+h \tag{II-101}$$

which implies that $T_q(x+h,\ h')=(h'/h)^{q+1}T_q(x+h,\ h)$ for any q. This then leads to a simple step-size dependence for $I_{\bar{q}}$ when combined with (II-99).

$$I_{\bar{q}}(x+h,\ h')=\left(\frac{h'}{h}\right)^{\bar{q}+1}I_{\bar{q}}(x+h,\ h) \tag{II-102}$$

If the integration error, in the sense of the norm, is to be ϵ^2, then we can define a step size $h'_{\bar{q}}$, for a method of order $\bar{q}$, by the equation

$$||I_{\bar{q}}(x+h,\ h'_{\bar{q}})||^2=\epsilon^2 \tag{II-103}$$

which can be readily solved for $h'_{\bar{q}}$.

$$\begin{aligned}\left(\frac{h'_{\bar{q}}}{h}\right)^{2(\bar{q}+1)}&=\left\{\gamma_{\bar{q}}^{-2(\bar{q}+1)}\left[\frac{||T_q(x+h,\ h)||^2}{||T_{\bar{q}}(x,\ \tilde{h})||^2}\right]||T_{\bar{q}}(x+h,\ h)/\epsilon||^2\right\}^{-1}\\&\equiv P_{\bar{q}}^{-2(\bar{q}+1)}\end{aligned} \tag{II-104}$$

The order of the method on the following integration step can be chosen as the one which permits the largest step size when calculated by equation (II-104), and the step size can be adjusted to the calculated value for that order.

The values of T_{q-1} and T_{q+1} required by equation (II-104) can be estimated in two ways. One is based on equation (II-100), while the other is based on equation (II-101). To apply equation (II-100), it is only necessary to express the derivatives appearing in it in terms of quantities calculable from the integration method. Thus we might write the identity

$$\frac{h^q y^{(q)}(x)}{q!}=\frac{h^q y^q(x+h)}{q!}-\frac{h^q[y^{(q)}(x+h)-y^{(q)}(x)]}{q!}$$

and the approximation

$$\frac{h^{q+1}y^{(q+1)}(x)}{(q+1)!} \cong \frac{h^{q+1}[y^{(q)}(x+h)-y^{(q)}(x)]}{h(q+1)!}$$

$$= \frac{h^{q}[y^{(q)}(x+h)-y^{(q)}(x)]}{q!(q+1)}$$

in place of the derivatives in equation (II-100).

$$T_{q-1}(x+h,\ h) = T_q(x+h,\ h) + \frac{h^q y^q(x+h)}{q!} - \frac{h^q[y^{(q)}(x+h)-y^{(q)}(x)]}{q!}$$

$$T_{q+1}(x+h,\ h) = T_q(x+h,\ h) - \frac{h^q[y^{(q)}(x+h)-y^{(q)}(x)]}{q!(q+1)} \tag{II-105}$$

The quantities appearing on the right side of these two expressions are all available at the conclusion of an integration step. Alternatively, to implement equation (II-101) in the calculation of T_{q-1} and T_{q+1}, it is possible to use the approximations

$$y^{(q)}(\xi) \cong \frac{[y^{(q)}(x+h)+y^{(q)}(x)]}{2}$$

$$y^{(q+2)}(\xi) \cong \frac{[y^{(q+1)}(\xi)-y^{(q+1)}(\xi-h)]}{h}$$

in the expressions for the truncation error. Then from equation (II-101)

$$T_{q-1}(x+h,\ h) = \frac{h^q y^{(q)}(x+h)}{q!} - \frac{h^q[y^{(q)}(x+h)-y^{(q)}(x)]}{(q!)2}$$

$$T_{q+1}(x+h,\ h) = \frac{h^{q+1}[y^{(q+1)}(\xi)-y^{(q+1)}(\xi-h)]}{(q+1)!(q+2)} = \frac{T_q(x+h,\ h)-T_q(x,\ h)]}{(q+2)} \tag{II-106}$$

and again all terms are available at the conclusion of a step. For the integration methods of Theorem III.2, with $\nu=1$, we can write

$$T_q(x+h,\ h) = \ell_0 z_{q+1}(x+h)$$

$$h^q[y^{(q)}(x+h)-y^{(q)}(x)]/q! = \ell_q z_{q+l}(x+h) \tag{II-107a}$$

where ℓ_0 and ℓ_q are the first and last components of the vector ℓ. There is a simple relationship between ℓ_0 and ℓ_q. Since $\ell = \alpha T u$, it can be seen from table I that $\ell_q/\ell_k = k!/q!$ and, since, for the $h\to\infty$ limit we are interested in $k=0$, we have $\ell_q/\ell_0 = 1/q!$ For the $h\to 0$ limit we are interested in $k=p\geq 1$ and so we have, using equation (II-98),

$$\frac{\ell_q}{\ell_0} = \frac{\ell_q}{\ell_p}\frac{\ell_p}{\ell_0} = \frac{q+1}{(q+1-p)!} \tag{II-107b}$$

where p is the order of the differential equation being integrated. The right side of equation (II-107b) is thus also valid in the limit $h\to\infty$ if p is set to zero. The expressions in equation (II-107) can be used in either equation (II-105) or (II-106) to estimate the truncation error and hence the integration error through equation (II-99).

There are many norms which could be used for calculating the length of the n-dimensional truncation vector, but any suitable norm should have two desirable features. First, it should reflect the relative importance of the various components of the solution vector y, and second, it should reflect the history of y and the changes occurring in y as integration proceeds. The second feature implies that the norm must evolve as integration proceeds. Suppose that on the k^{th} step of the integration we write

$$||T_q||^2 \equiv T_q^* C^{(k)} T_q \qquad k=0, 1, 2, \ldots \tag{II-108}$$

where $C^{(k)}$ is a positive definite matrix. Then the simplest possibility is to assume that $C^{(k)}$ is a diagonal matrix written as a product of two other diagonal matrices. If the trace of a matrix A is written as $Tr(A)$, then

$$\begin{aligned} C^{(k)} &= \frac{U^{(k)} E^{(k)}}{Tr(U^{(k)})} \\ U^{(k)} &= \operatorname{diag}\left(U_1^{(k)}, U_2^{(k)}, \ldots, U_n^{(k)}\right) \\ E^{(k)} &= \operatorname{diag}\left(E_1^{(k)}, E_2^{(k)}, \ldots, E_n^{(k)}\right) \end{aligned} \tag{II-109}$$

where the first factor characterizes the relative importance of the components of y and the second factor characterizes the history of y to that point. For the balance of this section $y^{(k)}$ will denote the value of the solution vector at the k^{th} step rather than its k^{th} derivative. One possibility for $U^{(k)}$ is simply the unit matrix. If y_i represents the i^{th} component of y and k_1, k_2 are two fixed integers such that $k_1 \leq k_2$ and $1 \leq k_1, k_2 \leq n$, then another possibility for $U^{(k)}$ is

$$U_i^{(k)} = \begin{cases} \dfrac{(k_2 - k_1 + 1)|y_i^{(k)}|}{\sum\limits_{j=k_1}^{k_2} |y_j^{(k)}|} & k_1 \leq i \leq k_2 \\ 1 & \text{otherwise} \end{cases} \tag{III-110}$$

For both choices one can easily calculate the trace of $U^{(k)}$.

$$Tr(U^{(k)}) = n \tag{II-111}$$

To specify $E^{(k)}$, first define

$$E_i^{(k)} \equiv \frac{1}{\left(Y_i^{(k)}\right)^2} \tag{II-112}$$

and then consider some possibilities for $Y_i^{(k)}$. An immediate possibility for the evolution of $Y_i^{(k)}$, and hence of $E_i^{(k)}$, is

$$Y_i^{(k+1)} = \max\left\{Y_i^{(k)}, \left|y_i^{(k+1)}\right|\right\} \tag{II-113}$$

which means $Y^{(k)}$ is nondecreasing and essentially is the maximum absolute value attained by the i^{th} component of y. If one wished to permit $Y_i^{(k)}$ to decrease as well as increase, then one could consider

$$Y_i^{(k+1)} = \begin{cases} 0.9\, Y_i^{(k)} + (0.1)\left|y_i^{(k+1)}\right| & \dot{y}_i^{(k)} y_i^{(k)} \geq 0 \text{ and } 10^{-5} \leq \left|y_i^{(k+1)}\right| \leq \dfrac{Y_i^{(k)}}{2} \\ \max\left\{Y_i^{(k)},\ \left|y_i^{(k+1)}\right|\right\} & \text{otherwise} \end{cases} \tag{II-114}$$

as one possibility. There are also two obvious choices for the initial values of $Y_i^{(k)}$.

$$Y_i^{(0)} = \begin{cases} \left|y_i^{(0)}\right| & y_i^{(0)} \neq 0 \\ 1 & y_i^{(0)} = 0 \end{cases} \tag{II-115}$$

$$Y_i^{(0)} = \begin{cases} \left|y_i^{(0)}\right| & y_i^{(0)} \neq 0 \\ \min\left\{1, y_{\min}\right\} & y_i^{(0)} = 0 \end{cases} \tag{II-116}$$

$$y_{\min} = \min\left\{\left|y_j^{(0)}\right| > 0,\ j = 1, 2, \ldots, n\right\}$$

All of the possibilities cited here lead to a positive definite matrix for $C^{(k)}$. The Hindmarsh program (ref. 11) uses the unit matrix for $U^{(k)}$ with equations (II-113) and (II-115) for the matrix $E^{(k)}$.

Conclusions

A broad class of multistep numerical integration schemes to solve the initial value problem associated with a system of ordinary differential equations has been proposed and studied in this chapter. These methods are not restricted to a system in normal form, nor do they require that the system be first order or even that each component of the solution satisfy the same order differential equation. They are applicable when the solution is a vector-valued function whose domain is the reals and whose range is a vector space over the real or complex field. The general class of methods includes a subclass which contains both Gear's method for first order systems of stiff equations and Nordsieck's method for p^{th} order systems of equations. The analysis has shown that the Gear method for stiff equations is not restricted to first order differential equations but is directly applicable to higher order equations. It has also been demonstrated that both the Gear and Nordsieck methods are independent of the linear, multistep methods.

Appendix – Generalized Inverse

The generalized (Moore-Penrose) inverse of a matrix, introduced by Penrose (ref. 20) and others, represents a generalization of the inverse of a nonsingular matrix. A substantial effort has been expended on the study of its properties and methods for its computation. For convenience this appendix lists those properties of the generalized inverse which are needed in this analysis of numerical integration methods.

A.1 The generalized inverse of matrix A is the matrix $A^\dagger$, which is the unique solution (ref. 20, Theorem 1) of

$$AA^\dagger A=A \tag{A1.1}$$

$$A^\dagger AA^\dagger=A^\dagger \tag{A1.2}$$

$$(AA^\dagger)^*=AA^\dagger \tag{A1.3}$$

$$(A^\dagger A)^*=A^\dagger A \tag{A1.4}$$

A2.1 $(A^*)^\dagger=(A^\dagger)^*$ (ref. 20, Lemma 1.2)

A2.2 If A is nonsingular, then $A^\dagger=A^{-1}$ (ref. 20, Lemma 1.3).

A2.3 If $A=A^*$ and $AA=A$, then $A^\dagger=A$ (ref. 20, Lemma 2.2).

A.3 If A is of full-column rank, then $A^\dagger=(A^*A)^{-1}A^*$ (ref. 21, Lemma 1.e).

A.4 $\left(\oplus\sum A_i\right)^\dagger=\oplus\sum A_i^\dagger$ and $(A_1\otimes A_2)^\dagger=A_1^\dagger\otimes A_2^\dagger$, are easily verified.

A.5 Rank $(A)=$ Rank $(A^\dagger)=$ Rank $(A^\dagger A)$ (ref. 20, Lemma 1.9).

A.6 Let A, B, and C be matrices. The equation $AXB=C$ will have a solution if and only if $AA^\dagger CB^\dagger B=C$ and the general solution is $X=A^\dagger CB^\dagger+Y-A^\dagger A\,YBB^\dagger$, where Y is an arbitrary matrix (ref. 20, Theorem 2).

TABLE I. - THE VECTORS t, u, AND Tu OF THEOREM III.1 AND THEOREM III.2 WHERE $t^* = e_k^*PT$, $T^{-1}PT = 1_{q+1} + J_{q+1}$, $u(\epsilon) = \epsilon^{-1}\Gamma^{\dagger}c$, and $\epsilon = 1$

[For each value of k the eigenvalues of the stability matrix were chosen as $\lambda_j = 0\ (0 \leq j \leq q - k)$, $\lambda_j = 1\ (q + 1 - k \leq j \leq q)$.]

q	Vector	k = 0
1	t* u* -(Tu)*	(1,1) (-1,-1) (1,1)
2	t* u* -(Tu)*	(1,3/2,1/2) (-1/4,-3/2,-1) (1,3/2,1/2)
3	t* u* -(Tu)*	(1,2,7/6,1/6) (1/6,-5/6,-2,-1) (1,11/6,1,1/6)
4	t* u* -(Tu)*	(1,1/4,25/12,5/8,1/24) (55/720,0,-5/3,-5/2,-1) (1,50/24,35/24,10/24,1/24)
5	t* u* -(Tu)*	(1,3,13/4,3/2,31/120,1/120) (-13/240,47/240,-1/2,-11/4,-3,-1) (1,274/120,225/120,85/120,15/120,1/120)
6	t* u* -(Tu)*	(1,7/2,14/3,35/12,301/360,7/80,1/720) (-247/8640,7/480,49/240,-70/48,-490/120,-7/2,-1) (1,1764/720,1624/720,735/720,175/720,21/720,1/720)
7	t* u* -(Tu)*	(1,4,19/3,5,81/40,23/60,127/5040,1/5040) (311/15120,-991/15120,29/180,-31/360,-3,-17/3,-4,-1) (1,13068/5040,13132/5040,6769/5040,1960/5040,322/5040,28/5040, 1/5040)
8	t* u* -(Tu)*	(1,9/2,33/4,63/8,331/800,37/32,605/4032,51/8064,1/40320) (4657/40320,-39/5040,-59/1260,5/16,-37/40,-21/4,-15/2,-9/2,-1) (1,109584/40320,118124/40320,67284/40320,22449/40320,4536/40320, 546/40320,36/40320,1/40320)
		k = 1
1	t* u* -(Tu)*	(0,1) (0,-1) (0,1)
2	t* u* -(Tu)*	(0,1,1) (0,-1,-1) (1/2,1,1/2)
3	t* u* -(Tu)*	(0,1,3/2,1/2) (0,-1/4,-3/2,1) (1/2,1,3/4,1/6)
4	t* u* -(Tu)*	(0,1,2,7/6,1/6) (0,1/6,-5/6,-2,-1) (23/72,1,11/12,1/3,1/24)
5	t* u* -(Tu)*	(0,1,5/2,25/12,5/8,1/24) (0,55/720,0,-5/3,-5/2,-1) (41/144,1,25/24,35/72,5/48,1/120)
6	t* u* -(Tu)*	(0,1,3,13/4,3/2,31/120,1/120) (0,-13/240,47/240,-1/2,-11/4,-3,-1) (157/480,1,137/120,5/8,17/96,1/40,1/720)
7	t* u* -(Tu)*	(0,1,7/2,14/3,70/24,301/360,7/80,1/720) (0,-1729/60480,7/480,49/240,-70/48,-49/12,-7/2,-1) (29/90,1,49/40,203/270,49/192,7/144,7/1440,1/5040)
8	t* u* -(Tu)*	(0,1,4,19/3,5,81/40,23/60,127/5040,1/5040) (0,311/15120,-991/15120,29/180,-31/36,-3,-17/3,-4,-1) (175451/604300,1,363/280,469/540,967/2880,7/90,23/2160,1/1260, 1/40320)
		k = 2
2	t* u* -(Tu)*	(0,0,1/2) (0,0,-2) (0,0,1)
3	t* u* -(Tu)*	(0,0,1/2,1/2) (0,0,-2,-2) (1/3,1,1,1/3)
4	t* u* -(Tu)*	(0,0,1/2,3/4,1/4) (0,0,-1/2,-3,-2) (5/12,1,1,1/2,1/12)
5	t* u* -(Tu)*	(0,0,1/2,1,7/12,1/12) (0,0,1/3,-10/6,-4,-2) (1/30,23/36,1,11/18,1/6,1/60)
6	t* u* -(Tu)*	(0,0,1/2,5/4,25/24,5/16,1/48) (0,0,11/72,0,-10/3,-5,-2) (-1/27,41/72,1,25/36,35/144,1/24,1/360)
7	t* u* -(Tu)*	(0,0,1/2,3/2,13/8,3/4,31/240,1/240) (0,0,-13/120,47/120,-1,-11/2,-6,-2) (207/1008,157/240,1,137/180,5/16,17/240,1/120,1/2520)
8	t* u* -(Tu)*	(0,0,1/2,7/4,7/3,35/24,301/720,7/160,1/1440) (0,0,-247/4320,7/240,49/120,-35/12,-49/6,-7,-2) (10277/43200,29/45,1,49/60,203/540,49/480,7/432,1/720,1/20160)
q	Vector	k = 3
3	t* u* -(Tu)*	(0,0,0,1/6) (0,0,0,-6) (0,0,0,1)
4	t* u* -(Tu)*	(0,0,0,1/6,1/6) (0,0,0,-6,-6) (1/4,1,3/2,1,1/4)
5	t* u* -(Tu)*	(0,0,0,1/6,1/4,1/12) (0,0,0,-3/2,-9,-6) (9/20,5/4,3/2,1,3/8,1/20)
6	t* u* -(Tu)*	(0,0,0,1/6,1/3,7/36,1/36) (0,0,0,1,-5,-12,-6) (-109/360,1,23/24,1,11/24,1/10,1/120)
7	t* u* -(Tu)*	(0,0,0,1/6,5/12,25/72,5/48,1/144) (0,0,0,11/24,0,-10,-15,-6) (-515/1008,-1/9,41/48,1,25/48,7/48,1/48,1/840)
8	t* u* -(Tu)*	(0,0,0,1/6,1/2,13/24,1/4,31/720,1/720) (0,0,0,-13/40,47/40,-3,-33/2,-18,-6) (12149/33600,69/112,157/160,1,137/240,3/16,17/480,1/280,1/6720)
		k = 4
4	t* u* -(Tu)*	(0,0,0,0,1/24) (0,0,0,0,-24) (0,0,0,0,1)
5	t* u* -(Tu)*	(0,0,0,0,1/24,1/24) (0,0,0,0,-24,-24) (1/5,1,2,2,1,1/5)
6	t* u* -(Tu)*	(0,0,0,0,1/24,5/80,1/48) (0,0,0,0,-6,-36,-24) (17/30,9/5,5/2,2,1,3/10,1/30)
7	t* u* -(Tu)*	(0,0,0,0,1/24,1/12,7/144,1/144) (0,0,0,0,4,-20,-48,-24) (-97/105,-109/90,1/5,23/18,1,11/30,1/15,1/210)
8	t* u* -(Tu)*	(0,0,0,0,1/24,5/48,25/288,5/192,1/576) (0,0,0,0,11/6,0,-40,-60,-24) (-577/360,-515/252,-2/9,41/36,1,5/12,7/72,1/84,1/1680)
		k = 5
5	t* u* -(Tu)*	(0,0,0,0,0,1/120) (0,0,0,0,0,-120) (0,0,0,0,0,1)
6	t* u* -(Tu)*	(0,0,0,0,0,1/120,1/120) (0,0,0,0,0,-120,-120) (1/6,1,5/2,10/3,5/2,1,1/6)
7	t* u* -(Tu)*	(0,0,0,0,0,1/120,1/80,1/240) (0,0,0,0,0,-30,-180,-120) (33/42,17/6,9/2,25/6,5/2,1,1/4,1/42)
8	t* u* -(Tu)*	(0,0,0,0,0,1/120,1/60,7/720,1/720) (0,0,0,0,0,20,-100,-240,-120) (-2257/1008,-97/21,-109/36,1/3,115/72,1,11/36,1/21,1/336)
		k = 6
6	t* u* -(Tu)*	(0,0,0,0,0,0,1/720) (0,0,0,0,0,0,-720) (0,0,0,0,0,0,1)
7	t* u* -(Tu)*	(0,0,0,0,0,0,1/720,1/720) (0,0,0,0,0,0,-720,-720) (1/7,1,3,5,5,3,1,1/7)
8	t* u* -(Tu)*	(0,0,0,0,0,0,1/720,1/480,1/1440) (0,0,0,0,0,0,-180,-1080,-720) (65/56,33/7,17/2,9,25/4,3,1,3/14,1/56)
		k = 7
7	t* u* -(Tu)*	(0,0,0,0,0,0,0,1/5040) (0,0,0,0,0,0,0,-5040) (0,0,0,0,0,0,0,1)
8	t* u* -(Tu)*	(0,0,0,0,0,0,0,1/5040,1/5040) (0,0,0,0,0,0,0,-5040,-5040) (1/8,1,7/2,7,35/4,7,7/2,1,1/8)
		k = 8
8	t* u* -(Tu)*	(0,0,0,0,0,0,0,0,1/40320) (0,0,0,0,0,0,0,0,-40320) (0,0,0,0,0,0,0,0,1)

TABLE II. - COEFFICIENTS FOR GEAR AND NORDSIECK INTEGRATION METHODS

(a) Gear method of polynomial degree q for a system of first order ordinary differential equations[a]

q	
1	(1,1)
2	(2/3,1,1/3)
3	(6/11,1,6/11,1/11)
4	(24/50,1,35/50,10/50,1/50)
5	(120/274,1,225/274,85/274,15/274,1/274)
6	(720/1764,1,1624/1764,735/1764,175/1764,21/1764,1/1764)

(b) Nordsieck method of polynomial degree q for a system of p^{th} order ordinary differential equations[b]

q	p = 1
1	(1/2,1)
2	(5/12,1,1/2)
3	(3/8,1,3/4,1/6)
4	(251/720,1,11/12,1/3,1/24)
5	(95/288,1,25/24,35/72,5/48,1/120)
6	(19087/60480,1,137/120,5/8,17/96,1/140,1/720)
7	(5257/17280,1,49/40,203/270,49/192,7/144,7/1440,1/5040)
	p = 2
2	(1/2)(1/3,1,1)
3	(1/2)(1/4,5/6,1,1/3)
4	(1/2)(19/90,3/4,1,1/2,1/12)
5	(1/2)(3/16,251/360,1,11/18,1/6,1/60)
6	(1/2)(863/5040,95/144,1,25/36,35/144,1/24,1/360)
7	(1/2)(275/1728,19087/30240,1,137/180,5/16,17/240,1/120,1/2520)
	p = 3
3	(1/3)(1/4,1,3/2,1)
4	(1/3)(7/40,3/4,5/4,1,1/4)
5	(1/3)(17/120,19/30,9/8,1,3/8,1/20)
6	(1/3)(41/336,9/16,251/240,1,11/24,1/10,1/120)
7	(1/3)(731/6720,863/1680,95/96,1,25/48,7/48,1/48,1/840)
8	(1/3)(8563/86400,275/576,19087/20160,1,137/240,3/16,17/480,1/280,1/6720)
	p = 4
4	(1/4)(1/5,1,2,2,1)
5	(1/4)(2/15,7/10,3/2,5/3,1,1/5)
6	(1/4)(11/105,17/30,19/15,3/2,1,3/10,1/30)
7	(1/4)(89/1008,41/84,9/8,251/180,1,11/30,1/15,1/210)
8	(1/4)(5849/75600,731/1680,863/840,95/72,1,5/12,7/72,1/84,1/1680)
9	(1/4)(1501/21600,8563/21600,275/288,19087/15120,1,137/300,1/8,17/840,1/560,1/15120)
	p = 5
5	(1/5)(1/6,1,5/12,10/3,5/2,1)
6	(1/5)(3/28,2/3,7/24,5/2,25/12,1,1/6)
7	(1/5)(83/1008,11/21,17/72,19/9,15/8,1,1/4,1/42)
8	(1/5)(59/864,445/1008,205/1008,15/8,251/144,1,11/36,1/21,1/336)
9	(1/5)(397/6720,5849/15120,731/4032,863/504,475/288,1,25/72,5/72,5/672,1/3024)
10	(1/5)(29939/570240,1501/4320,8563/51840,1375/864,19087/12096,1,137/360,5/56,17/1334,1/1008,1/756000)

[a] These numbers were taken from Gear's paper (ref. 7).

[b] The coefficients for ($p = 1$, $2 \le q \le 6$) were taken from Nordsieck (ref. 2), and those for ($p = 1$, $q = 7$) from Gear (ref. 3). The remaining coefficients were calculated from the formula $\ell_k = (p - 1)!(k - p + 1)!c_{k-p+1}/k!$ for $0 \le k \le q$ and by using the definition $k! = 1/(-k)!$ for $k < 0$. The numbers c_i were tabulated by LaBudde (ref. 5), and his indices M and s are related to p and q by the formulas $s = p - 1$, $M = q - p + 1$. Apart from the factor p^{-1}, these agree exactly with those given by Gear (ref. 3) for ($p = 2$, $4 \le q \le 7$) ($p = 3$, 4 _ q _ 7) and ($p = 4$, $5 \le q \le 7$) with the single exception of the third component for $p = 4$ and $q = 7$, where Gear gives 191/180 = 251/180 - 1/3 in place of 251/180.

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Chapter III

Numerical Details and Definitions of Cycle Performance Parameters

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In the first two chapters of this report I have discussed the theoretical aspects associated with the contruction of a mathematical model of the internal combustion engine. These included the governing differential equation, the modeling functions, and numerical integration schemes. It is true that these are the major structural underpinnings of a model, but a wide chasm separates them from a complete and usable model. This chasm must be bridged by the numerical details, which flesh out the model and translate it into a numerically functioning reality. I cannot possibly list the myriad minutiae which went into the implementation of the theoretical structure. Instead I shall concentrate on the pivotal features of the successful conversion of theory into numerics. This will include a listing of (1) the specific forms of the differential equations used in calculations, (2) the chosen integration methods, and (3) miscellaneous numerical techniques. I shall separately discuss the general model and each of its three specializations. The equations for these models were derived in Chapter I, but they will not be used directly in the derived form.

Equations for General Model

Differential Equations and Jacobians

The noncombustion phase of the cycle is described by equations for temperature, composition, and mass. These are obtainable from the equations given in Chapter I (eqs. (I-72), (I-73), (I-75), and (I-76)) and the thermodynamic relations (I-130) to (I-137).

$$
\begin{aligned}
\frac{dT}{d\theta} &= \dot{T} \equiv \left({}^{*}C^{\lambda} n_{\lambda}\right)^{-1} \Bigg(-\frac{p}{\rho}\frac{d \ln V}{d\theta} - \frac{{}^{*}U^{\lambda} R_{\lambda}}{\rho\omega} + M^{-1} \Bigg\{ \left[\tilde{h}^{(+)} - {}^{*}U^{\lambda} \tilde{n}_{\lambda}^{(+)}\right] \frac{dM^{(+)}}{d\theta} \\
&\qquad + \left[\tilde{h}^{(-)} - {}^{*}U^{\lambda} \tilde{n}_{\lambda}^{(-)}\right] \frac{dM^{(-)}}{d\theta} - \frac{\dot{Q}}{\omega} \Bigg\} \Bigg) \\
\frac{dn_{\lambda}}{d\theta} &= \dot{n}_{\lambda} \equiv \frac{R_{\lambda}}{\rho\omega} + M^{-1} \left\{ \left[\tilde{n}_{\lambda}^{(+)} - n_{\lambda}\right] \frac{dM^{(+)}}{d\theta} + \left[\tilde{n}_{\lambda}^{(-)} - n_{\lambda}\right] \frac{dM^{(-)}}{d\theta} \right\} \\
\frac{dM}{d\theta} &= \dot{M} \equiv \frac{dM^{(+)}}{d\theta} + \frac{dM^{(-)}}{d\theta}
\end{aligned}
\tag{III-1}
$$

The combustion phase of the cycle is described by equations for the temperature, composition, and mass of both the burned gas and the unburned gas. These equations are also obtainable from the equations given in Chapter I (eqs. (I-73), (I-74), (I-75), (I-77), (I-82), (I-83), and (I-123)) and the thermodynamic relations (I-130) to (I-137).

$$\frac{dn_\lambda^{(1)}}{d\theta} = \dot{n}_\lambda^{(1)} \equiv \frac{R_\lambda^{(1)}}{\rho_1\omega} + M_1^{-1}\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right]\dot{M}_1^{(-)} + \left[\tilde{n}_\lambda^{(1,b)} - n_\lambda^{(1)}\right]\left[\frac{d\ln M_1}{d\theta} - \frac{\dot{M}_1^{(-)}}{M_1}\right]$$

$$\frac{dT_1}{d\theta} = \dot{T}_1 \equiv \left[{}^*C_1^\lambda n_\lambda^{(1)}\right]^{-1}\left\{\frac{-p_1}{\rho_1}\frac{d\ln V_1}{d\theta} - \frac{{}^*U_1^\lambda R_\lambda^{(1)}}{\rho_1\omega} - \frac{\dot{Q}_1}{M_1\omega} + M_1^{-1}\left[\tilde{h}_1^{(-)} - {}^*U_1^\lambda\tilde{n}_\lambda^{(1,-)}\right]\dot{M}_1^{(-)}\right.$$
$$\left. + \left[\tilde{h}_1^{(b)} - {}^*U_1^\lambda\tilde{n}_\lambda^{(1,b)}\right]\left[\frac{d\ln M_1}{d\theta} - \frac{\dot{M}_1^{(-)}}{M_1}\right]\right\} \qquad \text{(III-2)}$$

$$\frac{dM_1}{d\theta} = \dot{M}_1 \equiv \dot{M}_b + \dot{M}_1^{(-)}$$

$$\frac{dT_2}{d\theta} = \dot{T}_2 \equiv \left[{}^*C_2^\lambda n_\lambda^{(2)}\right]^{-1}\left(\frac{p_2}{\rho_2}\frac{d\ln\rho_2}{d\theta} - \frac{\dot{Q}_2}{M_2\omega}\right)$$

There are, of course, also equations for the composition of the unburned gas, $dn_\lambda^{(2)}/d\theta = 0$, and its mass, $dM_2/d\theta = -\dot{M}_b$, which are trivially integrable. Thus the unburned-gas composition is constant, and its mass is given simply by $M_2(\theta) = M(\theta_0) - M_b(\theta)$. The differential equations (III-2) are supplemented with the pair of simultaneous linear equations (I-78) and (I-82), which determine $d\ln V_1/d\theta$ and $d\ln V_2/d\theta$. Because equation (I-82) is trivial, it will not be repeated. The other member of the pair, equation (I-78), can be cast into a relatively simple form.

$$-\left(\frac{\partial\ln p_1}{\partial\ln\rho_1} + \frac{p_1}{\rho_1}\frac{\partial\ln p_1}{\partial u_1}\right)\frac{d\ln V_1}{d\theta} + \left(\frac{\partial\ln p_2}{\partial\ln\rho_2} + \frac{p_2}{\rho_2}\frac{\partial\ln p_2}{\partial u_2}\right)\frac{d\ln V_2}{d\theta}$$
$$= \left(\frac{\partial\ln p_2}{\partial\ln\rho_2} + \frac{p_2}{\rho_2}\frac{\partial\ln p_2}{\partial u_2}\right)\frac{d\ln M_2}{d\theta} - \frac{\dot{Q}_2}{M_2\omega}\frac{\partial\ln p_2}{\partial u_2}$$
$$-\left(\frac{\partial\ln p_1}{\partial\ln\rho_1} + \frac{p_1}{\rho_1}\frac{\partial\ln p_1}{\partial u_1}\right)\frac{d\ln M_1}{d\theta} + \left[\frac{\dot{Q}_1}{M_1\omega} - (h_2 - h_1)\frac{d\ln M_1}{d\theta}\right]\frac{\partial\ln p_1}{\partial u_1}$$
$$-\frac{\partial\ln p_1}{\partial n_\lambda^{(1)}}\frac{dn_\lambda^{(1)}}{d\theta} - \frac{\partial\ln p_1}{\partial u_1}\left(\tilde{h}_1^{(-)} - h_2\right)\frac{\dot{M}_1^{(-)}}{M_1} \qquad \text{(III-3a)}$$

The partial derivatives in this equation are to be interpreted as

$$\frac{\partial\ln p_1}{\partial\ln\rho_1} + \frac{p_1}{\rho_1}\frac{\partial\ln p_1}{\partial u_1} = \left(\frac{\partial\ln p_1}{\partial\ln\rho_1}\right)_{u_1,n_\lambda^{(1)}} + \frac{p_1}{\rho_1}\left(\frac{\partial\ln p_1}{\partial u_1}\right)_{\rho_1,n_\lambda^{(1)}}$$

$$\frac{\partial\ln p_2}{\partial\ln\rho_2} + \frac{p_2}{\rho_2}\frac{\partial\ln p_2}{\partial u_2} = \left(\frac{\partial\ln p_2}{\partial\ln\rho_2}\right)_{u_2,n_\lambda^{(2)}} + \frac{p_2}{\rho_2}\left(\frac{\partial\ln p_2}{\partial u_2}\right)_{\rho_2,n_\lambda^{(2)}} = \left(\frac{\partial\ln p_2}{\partial\ln\rho_2}\right)_{s_2,n_\lambda^{(2)}} \equiv \gamma_2 \qquad \text{(III-3b)}$$

$$\frac{\partial\ln p_1}{\partial u_1} = \left(\frac{\partial\ln p_1}{\partial u_1}\right)_{\rho_1,n_\lambda^{(1)}}, \quad \frac{\partial\ln p_2}{\partial u_2} = \left(\frac{\partial\ln p_2}{\partial u_2}\right)_{\rho_2,n_\lambda^{(2)}}, \quad \frac{\partial\ln p_1}{\partial n_\lambda^{(1)}} = \left(\frac{\partial\ln p_1}{\partial n_\lambda^{(1)}}\right)_{u_1,\rho_1}$$

where the derivatives on the right are evaluated by using equations (I-136) and (I-137).

To integrate the differential equations (III-1) and (III-2) numerically, it is necessary to know their Jacobian matrices, the derivatives of the right side with respect to the dependent variables. To calculate the Jacobian of equation (III-1), I shall use $p/\rho = RT\sum_\lambda n_\lambda$ (eq. (I-132)), and $\rho = M/V$ (eq. (I-75)), whose derivatives are quite simple.

$$\frac{\partial(p/\rho)}{\partial T}=R\sum_{\lambda}n_{\lambda},\qquad \frac{\partial(p/\rho)}{\partial n_{\mu}}=RT,\qquad \frac{\partial(p/\rho)}{\partial M}=0$$

$$\frac{\partial \ln \rho}{\partial T}=0,\qquad \frac{\partial \ln \rho}{\partial n_{\mu}}=0,\qquad \frac{\partial \ln \rho}{\partial M}=M^{-1} \tag{III-4}$$

I shall also use

$$\frac{\partial \dot{M}^{(\pm)}}{\partial n_{\mu}}\cong 0,\qquad \frac{\partial \dot{M}^{(\pm)}}{\partial T}\cong 0,\qquad \frac{\partial \dot{M}^{(\pm)}}{\partial M}=0$$

$$\frac{\partial \dot{Q}}{\partial n_{\mu}}\cong 0,\qquad \frac{\partial \dot{Q}}{\partial T}\cong \bar{h}A,\qquad \frac{\partial \dot{Q}}{\partial M}=0 \tag{III-5}$$

with the first two of each triplet in this equation being approximations to the exact derivatives. The derivatives in equations (III–4) and (III–5) lead to the following Jacobian matrix for system (III–1):

$$\frac{\partial \dot{n}_{\lambda}}{\partial n_{\mu}}=\frac{1}{\rho\omega}\frac{\partial R_{\lambda}}{\partial n_{\mu}}+M^{-1}\left\{\frac{\partial\left[\tilde{n}_{\lambda}^{(\pm)}-n_{\lambda}\right]}{\partial n_{\mu}}\frac{dM^{(+)}}{d\theta}+\frac{\partial\left[\tilde{n}_{\lambda}^{(-)}-n_{\lambda}\right]}{\partial n_{\mu}}\frac{dM^{(-)}}{d\theta}\right\}$$

$$\frac{\partial \dot{n}_{\lambda}}{\partial T}=\frac{1}{\rho\omega}\frac{\partial R_{\lambda}}{\partial T},\qquad \frac{\partial \dot{n}_{\lambda}}{\partial M}=\frac{-\dot{n}_{\lambda}}{M}$$

$$\begin{aligned}\frac{\partial \dot{T}}{\partial n_{\mu}}=\left({}^{*}C^{\tau}n_{\tau}\right)^{-1}\Bigg(&-{}^{*}C^{\mu}\dot{T}-RT\frac{d\ln V}{d\theta}-\frac{{}^{*}U^{\lambda}}{\rho\omega}\frac{\partial R_{\lambda}}{\partial n_{\mu}}\\&+M^{-1}\left\{\frac{\partial\left[\tilde{h}^{(+)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(+)}\right]}{\partial n_{\mu}}\frac{dM^{(+)}}{d\theta}+\frac{\partial\left[\tilde{h}^{(-)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(-)}\right]}{\partial n_{\mu}}\frac{dM^{(-)}}{d\theta}\right\}\Bigg)\end{aligned}$$

$$\begin{aligned}\frac{\partial \dot{T}}{\partial T}=\left({}^{*}C^{\tau}n_{\tau}\right)^{-1}\Bigg(&-{}^{*}\dot{C}^{\lambda}n_{\lambda}\dot{T}-R\sum_{\lambda}n_{\lambda}\frac{d\ln V}{d\theta}-\frac{1}{\rho\omega}\left({}^{*}C^{\lambda}R_{\lambda}+{}^{*}U^{\lambda}\frac{\partial R_{\lambda}}{\partial T}\right)-\frac{\bar{h}A}{M\omega}\\&+M^{-1}\left\{\frac{\partial\left[\tilde{h}^{(+)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(+)}\right]}{\partial T}\frac{dM^{(+)}}{d\theta}+\frac{\partial\left[\tilde{h}^{(-)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(-)}\right]}{\partial T}\frac{dM^{(-)}}{d\theta}\right\}\Bigg)\end{aligned} \tag{III-6}$$

$$\begin{aligned}\frac{\partial \dot{T}}{\partial M}=\left({}^{*}C^{\tau}n_{\tau}\right)^{-1}\Bigg(&M^{-1}\frac{{}^{*}U^{\lambda}R_{\lambda}}{\rho\omega}-M^{-2}\Bigg\{\left[\tilde{h}^{(+)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(+)}\right]\frac{dM^{(+)}}{d\theta}\\&+\left[\tilde{h}^{(-)}-{}^{*}U^{\lambda}\tilde{n}_{\lambda}^{(-)}\right]\frac{dM^{(-)}}{d\theta}-\frac{\dot{Q}}{\omega}\Bigg\}\Bigg)=-\frac{\dot{T}}{M}-\frac{\left({}^{*}C^{\lambda}n_{\lambda}\right)^{-1}\left(\frac{p}{\rho}\frac{d\ln V}{d\theta}\right)}{M}\end{aligned}$$

$$\frac{\partial \dot{M}}{\partial n_{\mu}}=0,\qquad \frac{\partial \dot{M}}{\partial T}=0,\qquad \frac{\partial \dot{M}}{\partial M}=0$$

The derivatives of R_{λ} which appear in these expressions are given by equations (I–148) and (I–151). The remaining derivatives have simple forms.

$$
\begin{gathered}
{}^*\dot{C}^{\lambda} = \frac{d^2\,{}^*U^{\lambda}}{dT^2} = \frac{d\,{}^*C^{\lambda}}{dT} \\
\frac{\partial\left[\tilde{h}^{(\pm)} - {}^*U^{\lambda}\tilde{n}_{\lambda}^{(\pm)}\right]}{\partial T} = \begin{cases} R\sum\limits_{\lambda} n_{\lambda} & \dfrac{dM^{(\pm)}}{d\theta} < 0 \\ -\,{}^*C^{\lambda}\tilde{n}_{\lambda}^{(\pm)} & \dfrac{dM^{(\pm)}}{d\theta} \geq 0 \end{cases} \\
\frac{\partial\left[\tilde{h}^{(\pm)} - {}^*U^{\lambda}\tilde{n}_{\lambda}^{(\pm)}\right]}{\partial n_{\mu}} = \begin{cases} RT & \dfrac{dM^{(\pm)}}{d\theta} < 0 \\ 0 & \dfrac{dM^{(\pm)}}{d\theta} \geq 0 \end{cases} \\
\frac{\partial\left[\tilde{n}_{\lambda}^{(\pm)} - n_{\lambda}\right]}{\partial n_{\mu}} = \begin{cases} 0 & \dfrac{dM^{(\pm)}}{d\theta} < 0 \\ -\delta_{\lambda}^{\mu} & \dfrac{dM^{(\pm)}}{d\theta} \geq 0 \end{cases}
\end{gathered}
\qquad \text{(III-7)}
$$

To calculate the Jacobian matrix for the equations of the combustion phase, it is necessary to know some derivatives in addition to those used to calculate the Jacobian for the noncombustion phase. From the first member of equation (I-83), the equation of state (eq. (I-132)), and the equality of pressure (second last member of eq. (I-77)) one can obtain an expression for ρ_1.

$$
\rho_1 = \frac{M_1}{V_1} = M_1 V^{-1}\left[1 + \left(M_2 T_2 \sum_{\lambda} n_{\lambda}^{(2)} \Big/ M_1 T_1 \sum_{\tau} n_{\tau}^{(1)}\right)\right] \qquad \text{(III-8)}
$$

From this expression it is easy to calculate the derivatives of ρ_1.

$$
\begin{gathered}
\frac{\partial \ln \rho_1}{\partial \ln T_1} = -\left[\mathrm{M}_2 T_2 \sum_{\lambda} n_{\lambda}^{(2)} \Big/ M_1 T_1 \sum_{\tau} n_{\tau}^{(1)}\right]\left[1 + \left(M_2 T_2 \sum_{\lambda} n_{\lambda}^{(2)} \Big/ M_1 T_1 \sum_{\tau} n_{\tau}^{(1)}\right)\right]^{-1} \\
\frac{\partial \ln \rho_1}{\partial \ln T_2} = -\frac{\partial \ln \rho_1}{\partial \ln T_1} \\
\frac{\partial \ln \rho_1}{\partial n_{\mu}^{(1)}} = \frac{\partial \ln \rho_1}{\partial \ln T_1}\left(\sum_{\lambda} n_{\lambda}^{(1)}\right)^{-1} \\
\frac{\partial \ln \rho_1}{\partial \ln M_1} = \left[1 + \left(M_2 T_2 \sum_{\lambda} n_{\lambda}^{(2)} \Big/ M_1 T_1 \sum_{\tau} n_{\tau}^{(1)}\right)\right]^{-1}
\end{gathered}
\qquad \text{(III-9)}
$$

It will also be convenient to rewrite a term that appears as part of the differential equation for T_1 in equation (III-2) to facilitate the calculation of its derivatives.

$$\tilde{h}_1^{(-)} - {}^*U_1^\lambda \tilde{n}_\lambda^{(1,-)} = (h_1 - u_1) + \left\{\tilde{h}_1^{(-)} - h_1 - {}^*U_1^\lambda\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right]\right\}$$

$$= \frac{p_1}{\rho_1} + \left\{\tilde{h}_1^{(-)} - h_1 - {}^*U_1^\lambda\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right]\right\}$$

The term $\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right]$, which appears on the right and also in the composition equations in the set of differential equation (III-2), is identically zero when $\dot{M}_1^{(-)} < 0$. Thus quantities involving it can contribute to the Jacobian only for $\dot{M}_1^{(-)} > 0$; but if this occurs, $\dot{M}_1^{(-)}$ will generally be relatively small and the contributions to the Jacobian will probably be negligible. The Jacobian matrix for the system (III-2) will be calculated on the basis of the assumption that a number of terms have zero derivatives.

$$\frac{\partial}{\partial n_\mu^{(1)}}\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right] = \frac{\partial}{\partial T_1}\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right] = \frac{\partial}{\partial M_1}\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right] = \frac{\partial}{\partial T_2}\left[\tilde{n}_\lambda^{(1,-)} - n_\lambda^{(1)}\right] = 0$$

$$\frac{\partial}{\partial n_\mu^{(1)}}\left\{\tilde{h}_1^{(-)} - h_1 - \left[{}^*U_1^\lambda \tilde{n}_\lambda^{(1,-)} - u_1\right]\right\} = \frac{\partial}{\partial T_1}\left\{\tilde{h}_1^{(-)} - h_1 - \left[{}^*U_1^\lambda \tilde{n}_\lambda^{(1,-)} - u_1\right]\right\}$$

$$= \frac{\partial}{\partial M_1}\left\{\tilde{h}_1^{(-)} - h_1 - \left[{}^*U_1^\lambda \tilde{n}_\lambda^{(1,-)} - u_1\right]\right\} = \frac{\partial}{\partial T_2}\left\{\tilde{h}_1^{(-)} - h_1 - \left[{}^*U_1^\lambda \tilde{n}_\lambda^{(1,-)} - u_1\right]\right\} = 0$$

$$\frac{\partial}{\partial n_\mu^{(1)}}\left(\frac{d \ln V_1}{d\theta}\right) = \frac{\partial}{\partial T_1}\left(\frac{d \ln V_1}{d\theta}\right) = \frac{\partial}{\partial M_1}\left(\frac{d \ln V_1}{d\theta}\right) = \frac{\partial}{\partial T_2}\left(\frac{d \ln V_1}{d\theta}\right) = 0$$

$$\frac{\partial}{\partial n_\mu^{(1)}}\left(\frac{d \ln \rho_2}{d\theta}\right) = \frac{\partial}{\partial T_1}\left(\frac{d \ln \rho_2}{d\theta}\right) = \frac{\partial}{\partial M_1}\left(\frac{d \ln \rho_2}{d\theta}\right) = \frac{\partial}{\partial T_2}\left(\frac{d \ln \rho_2}{d\theta}\right) = 0 \qquad \text{(III-10)}$$

$$\frac{\partial \tilde{n}_\lambda^{(1,b)}}{\partial n_\mu^{(1)}} = \frac{\partial \tilde{n}_\lambda^{(1,b)}}{\partial T_1} = \frac{\partial \tilde{n}_\lambda^{(1,b)}}{\partial M_1} = \frac{\partial \tilde{n}_\lambda^{(1,b)}}{\partial T_2} = 0$$

$$\frac{\partial \dot{M}_1^{(-)}}{\partial n_\mu^{(1)}} = \frac{\partial \dot{M}_1^{(-)}}{\partial T_1} = \frac{\partial \dot{M}_1^{(-)}}{\partial M_1} = \frac{\partial \dot{M}_1^{(-)}}{\partial T_2} = 0, \qquad \frac{\partial \dot{M}_b}{\partial n_\mu^{(1)}} = \frac{\partial \dot{M}_b}{\partial T_1} = \frac{\partial \dot{M}_b}{\partial M_1} = \frac{\partial \dot{M}_b}{\partial T_2} = 0$$

The differentiation of equation (III-2), combined with equation (III-10), produces the expressions used to evaluate the elements of the Jacobian matrix for the combustion phase of the cycle.

$$\frac{\partial \dot{n}_\lambda^{(1)}}{\partial n_\mu^{(1)}} = \frac{1}{\rho_1\omega}\left[\frac{\partial R_\lambda^{(1)}}{\partial n_\mu^{(1)}} - R_\lambda^{(1)}\frac{\partial \ln \rho_1}{\partial n_\mu^{(1)}}\right] - \delta_\lambda^\mu\left[\frac{d \ln M_1}{d\theta} - \frac{\dot{M}_1^{(-)}}{M_1}\right], \quad \frac{\partial \dot{n}_\lambda^{(1)}}{\partial T_1} = \frac{1}{\rho_1\omega}\left[\frac{\partial R_\lambda^{(1)}}{\partial T_1} - \frac{R_\lambda^{(1)}}{T_1}\frac{\partial \ln \rho_1}{\partial \ln T_1}\right]$$

$$\frac{\partial \dot{n}_\lambda^{(1)}}{\partial M_1} = -\frac{\dot{n}_\lambda^{(1)}}{M_1} + \left(1 - \frac{\partial \ln \rho_1}{\partial \ln M_1}\right)\frac{R_\lambda^{(1)}}{\rho_1\omega M_1}, \qquad \frac{\partial \dot{n}_\lambda^{(1)}}{\partial T_2} = -\frac{R_\lambda^{(1)}}{\rho_1\omega T_1}\frac{\partial \ln \rho_1}{\partial \ln T_2}$$

$$\frac{\partial \dot{T}_1}{\partial n_\mu^{(1)}} = -\left[{}^*C_1^\lambda n_\lambda^{(1)}\right]^{-1}\left\{\dot{T}_1{}^*C_1^\mu + RT_1\frac{d \ln V_1}{d\theta} + \frac{{}^*U_1^\lambda}{\rho_1\omega}\left[\frac{\partial R_\lambda^{(1)}}{\partial n_\mu^{(1)}} - R_\lambda^{(1)}\frac{\partial \ln \rho_1}{\partial n_\mu^{(1)}}\right] - \frac{RT_1\dot{M}_1^{(-)}}{M_1}\right\}$$

$$\begin{aligned}\frac{\partial \dot{T}_1}{\partial T_1} = -\left[{}^*C_1^\lambda n_\lambda^{(1)}\right]^{-1}\Bigg\{&{}^*\dot{C}_1^\lambda n_\lambda^{(1)}\dot{T}_1 + R\sum_\lambda n_\lambda^{(1)}\frac{d \ln V_1}{d\theta} + \frac{\bar{h}_1 A_1}{M_1\omega}\\ &+ \frac{1}{\rho_1\omega}\left({}^*U_1^\lambda\left[\frac{\partial R_\lambda^{(1)}}{\partial T_1} - \frac{R_\lambda^{(1)}}{T_1}\frac{\partial \ln \rho_1}{\partial \ln T_1}\right] + {}^*C_1^\lambda R_\lambda^{(1)}\right)\\ &- \frac{R\sum_\lambda n_\lambda^{(1)}\dot{M}_1^{(-)}}{M_1} + {}^*C_1^\lambda \tilde{n}_\lambda^{(1,b)}\left[\frac{d \ln M_1}{d\theta} - \frac{\dot{M}_1^{(-)}}{M_1}\right]\Bigg\}\end{aligned} \tag{III-11}$$

$$\frac{\partial \dot{T}_1}{\partial M_1} = -\frac{\dot{T}_1}{M_1} + \frac{\left[{}^*C_1^\lambda n_\lambda^{(1)}\right]^{-1}}{M_1}\left\{\frac{{}^*U_1^\lambda R_\lambda^{(1)}}{\rho_1\omega}\left(\frac{\partial \ln \rho_1}{\partial \ln M_1} - 1\right) - \frac{p_1}{\rho_1}\frac{d \ln V_1}{d\theta}\right\}$$

$$\frac{\partial \dot{T}_1}{\partial T_2} = \left[{}^*C_1^\lambda n_\lambda^{(1)}\right]^{-1}\left\{\frac{{}^*U_1^\lambda R_\lambda^{(1)}}{\rho_1\omega T_2}\frac{\partial \ln \rho_1}{\partial \ln T_2} + \left(\frac{\partial h_2}{\partial T_2}\right)\left[\frac{d \ln M_1}{d\theta} - \frac{\dot{M}_1^{(-)}}{M_1}\right]\right\}$$

$$\frac{\partial \dot{M}_1}{\partial n_\mu^{(1)}} = \frac{\partial \dot{M}_1}{\partial T_1} = \frac{\partial \dot{M}_1}{\partial M_1} = \frac{\partial \dot{M}_1}{\partial T_2} = 0, \qquad \frac{\partial \dot{T}_2}{\partial n_\mu^{(1)}} = \frac{\partial \dot{T}_2}{\partial T_1} = \frac{\partial \dot{T}_2}{\partial M_1} = 0$$

$$\frac{\partial \dot{T}_2}{\partial T_2} = -\left[{}^*C_2^\lambda n_\lambda^{(2)}\right]^{-1}\left[{}^*\dot{C}_2^\lambda n_\lambda^{(2)}\dot{T}_2 - R\sum_\lambda n_\lambda^{(2)}\frac{d \ln \rho_2}{d\theta} + \frac{\bar{h}_2 A_2}{M_2\omega}\right]$$

Extrapolation and Quadrature

During the integration of the differential equations over any portion of a cycle with intake or exhaust valve open, it is desirable to anticipate the crankangle location of those points where the mass flow rate reverses direction. These points correspond to zero mass flow rate through the intake or exhaust system $[\dot{M}^{(\pm)}=0]$ and have a bearing on the functions defined in equations (I-121) and (I-122). They occur when the cylinder pressure equals the manifold or exhaust pressure. One also needs to know where $M^{(\pm)}=0$. The estimated location of such points is calculable only by an extrapolation from previously calculated points. We have chosen to extrapolate with a cubic polynomial in both cases. Suppose we wish to approximate a function $f(\theta)$ in the vicinity of the point $\theta=\theta_1$ with a cubic polynomial in $\Delta\theta=\theta-\theta_1$ (fig. 1).

$$f(\theta)=a+b\,\Delta\theta+c(\Delta\theta)^2+d(\Delta\theta)^3 \tag{III-12}$$

Furthermore suppose we know both the value of f and its slope $\dot{f}=df/d\theta$ at θ_1 and $\theta_2=\theta_1-h$.

$$f(\theta_1)=f_1, \quad \dot{f}(\theta_1)=\dot{f}_1, \quad f(\theta_2)=f_2, \quad \dot{f}(\theta_2)=\dot{f}_2 \tag{III-13}$$

Then the coefficients a, b, c, and d can be determined so that the polynomial agrees with these values. Some simple algebra gives expressions for these coefficients in terms of the values at θ_1 and θ_2.

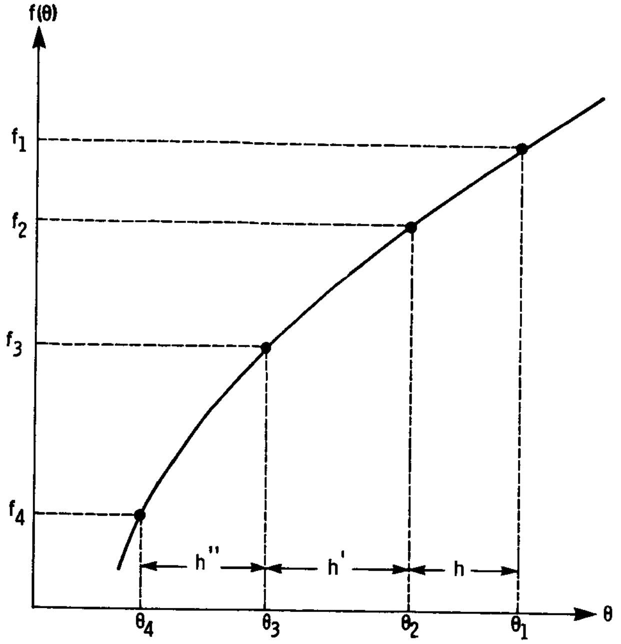


Figure 1. - Polynomial approximation as a function of crankangle.

$$a=f_1, \quad b=\dot{f}_1, \quad c=\frac{[3(f_2-f_1)/h+\dot{f}_2+2\dot{f}_1]}{h}, \quad d=\frac{[2(f_2-f_1)/h+\dot{f}_2+\dot{f}_1]}{h^2} \tag{III-14}$$

During a cycle calculation it is also necessary to carry out quadratures on various functions of θ. For example, the calculation of work is one such quadrature, and the evaluation of the function $\bar{\psi}^{(\pm)}$ (eq. (I-120)) is another. A cubic polynomial similar to equation (III-12) can be the basis for a quadrature formula, and it is convenient to center the polynomial on the point θ_2 rather than θ_1. Let $\overline{\Delta\theta}=\theta-\theta_2$ and

$$f(\theta)=\bar{a}+\bar{b}\,\overline{\Delta\theta}+\bar{c}(\overline{\Delta\theta})^2+\bar{d}(\overline{\Delta\theta})^3 \tag{III-15}$$

The values of f and its slope at θ_1 and θ_2 determine the coefficients of the polynomial.

$$\bar{a}=f_2, \quad \bar{b}=\dot{f}_2, \quad \bar{c}=\frac{[3(f_1-f_2)/h-(2\dot{f}_2+\dot{f}_1)]}{h}, \quad \bar{d}=\frac{[2(f_2-f_1)/h+\dot{f}_2+\dot{f}_1]}{h^2} \tag{III-16}$$

If we define the integral of $f(\theta)$ from $\theta=\theta_2$ to θ as

$$\Delta I \equiv \int_{\theta_2}^{\theta} f(z)\ dz \tag{III-17}$$

then from equation (III-15) we obtain the quadrature formula

$$\frac{\Delta I}{\overline{\Delta\theta}}=\bar{a}+\frac{\bar{b}}{2}\overline{\Delta\theta}+\frac{\bar{c}}{3}(\overline{\Delta\theta})^2+\frac{\bar{d}}{4}(\overline{\Delta\theta})^3 \tag{III-18}$$

and for $\overline{\Delta\theta}=h$ this reduces to a very simple result.

$$\frac{\Delta I}{h}=\frac{(f_1+f_2)}{2}+\frac{h(\dot{f}_2-\dot{f}_1)}{12} \tag{III-19}$$

Suppose that

$$f = p\frac{dV}{d\theta}, \quad \dot{f} = p\frac{d^2V}{d\theta^2} + \left(\frac{dp}{d\theta}\right)\left(\frac{dV}{d\theta}\right) \tag{III-20}$$

then both f and $\dot{f}$ are readily evaluated and ΔI is the work done by the working fluid over the crankangle interval $\Delta\theta$, while $\Delta I/\Delta\theta$ represents the average rate of work over the same interval. In this case it is possible to calculate f and $\dot{f}$ exactly because $dV/d\theta$ and $d^2V/d\theta^2$ can be calculated by differentiation of equation (I-86) and $dp/d\theta$ is obtained by a differentiation of the equation of state (eq. I-132)).

$$\frac{dV}{d\theta} = \frac{V(0)(r-1)\sin\theta}{2}[1 + (1 - \epsilon^2 \sin^2\theta)^{-1/2}\,\epsilon\cos\theta]$$

$$\frac{d^2V}{d\theta^2} = \frac{V(0)(r-1)}{2}\left[\cos\theta + (1 - \epsilon^2\sin^2\theta)^{-1/2}\,\epsilon\cos 2\theta + \frac{(1 - \epsilon^2\sin^2\theta)^{-3/2}\,\epsilon^3\sin^2 2\theta}{2}\right] \tag{III-21}$$

$$\frac{d\ln p}{d\theta} = \frac{d\ln\rho}{d\theta} + \frac{d\ln T}{d\theta} + \left(\sum_\tau n_\tau\right)^{-1}\sum_\lambda \frac{dn_\lambda}{d\theta}$$

In other cases it is not always possible to calculate $\dot{f}$ exactly. For example, associated with equation (I-120) we have integrands for which

$$f = g\dot{M}^{(\pm)}$$

$$\dot{f} = \dot{g}\dot{M}^{(\pm)} + g\ddot{M}^{(\pm)}$$

where g is some function of θ. In this case $\dot{f}$ cannot be calculated exactly since $\ddot{M}^{(\pm)}$ cannot be calculated exactly. To approximate $\ddot{M}^{(\pm)}$, we shall use

$$\ddot{M}_1^{(\pm)} = \ddot{M}_2^{(\pm)} = \frac{(\dot{M}_1^{(\pm)} - \dot{M}_2^{(\pm)})}{h} \tag{III-22}$$

where the subscripts on $\dot{M}^{(\pm)}$ and $\ddot{M}^{(\pm)}$ designate the two values of θ used in the evaluation. When $g = 1$, ΔI represents the increment in $M^{(\pm)}$, $\Delta M^{(\pm)}$, and equation (III-19) gives a very simple value for the increment in one integration step.

$$\frac{\Delta M^{(\pm)}}{h} = \frac{(\dot{M}_1^{(\pm)} + \dot{M}_2^{(\pm)})}{2} \tag{III-23}$$

There are situations where even $\dot{g}$ must be approximated. This is the case where g is the downstream enthalpy for flow out of the cylinder. Under these circumstances we approximate $\dot{g}$ similarly to the approximation for $\ddot{M}^{(\pm)}$

$$\dot{g}_1 = \dot{g}_2 = \frac{(g_1 - g_2)}{h} \tag{III-24}$$

To evaluate the heat transfer during the cycle, we must integrate $\dot{Q}/\omega$. Since $\dot{Q}$ is not easily obtained, we could calculate the quadrature of $\dot{Q}/\omega$ in a manner identical to that used for $\dot{M}^{(\pm)}$, which resulted in the approximation (III-23). I have chosen to proceed in a somewhat different manner. Suppose that the integrand f is again represented by a cubic polynomial centered on θ_1.

$$f(\theta) = \tilde{a} + \tilde{b}\,\Delta\theta + \tilde{c}(\Delta\theta)^2 + \tilde{d}(\Delta\theta)^3 \tag{III-25}$$

where the coefficients are to be determined by the values of f at four points as shown in figure 1. Then the cofficients can be obtained recursively.

$$-\tilde{d}(h' + \mathrm{h}'') = \frac{1}{h''}\left(\frac{f_4 - f_1}{h + h' + h''} - \frac{f_3 - f_1}{h + h'}\right) - \frac{1}{h'}\left(\frac{f_3 - f_1}{h + h'} - \frac{f_2 - f_1}{h}\right)$$

$$\tilde{c} - (2h + h')\tilde{d} = \frac{1}{h'}\left(\frac{f_3 - f_1}{h + h'} - \frac{f_2 - f_1}{h}\right), \qquad -\tilde{b} + h\tilde{c} - h^2\tilde{d} = \frac{(f_2 - f_1)}{h}, \qquad \tilde{a} = f_1 \tag{III-26}$$

The substitution of equation (III-25) into equation (III-17) with $\theta = \theta_1$ gives

$$\frac{\Delta I}{h} \equiv \frac{1}{h}\int_{\theta_2}^{\theta_1} f(\theta)\,d\theta = \tilde{a} - \frac{\tilde{b}h}{2} + \frac{\tilde{c}h^2}{3} - \frac{\tilde{d}h^3}{4} \tag{III-27}$$

This result could also have been used to calculate $M^{(\pm)}$, but we have found equation (III-23) to be adequate. When only two values of f are available, $\tilde{d}$ and $\tilde{c}$ are set to zero; if three values are known, only $\tilde{d}$ is set to zero.

The polynomials for extrapolation and quadrature, as well as any other polynomials used in calculations, are evaluated by nesting terms. For example, a cubic becomes

$$a_0 + a_1x + a_2x^2 + a_3x^3 = [(a_3x + a_2)x + a_1]x + a_0$$

and the form on the right tends to minimize numerical inaccuracy and computation time.

Chemistry Considerations

Both the combustion and noncombustion phases of the cycle are governed by equations which contain terms coming from the rate expressions of chemical kinetics. However, as a practical matter, chemical kinetics begins to play a substantial role in the cycle only with the onset of combustion at $\theta = \theta_0$. As the cycle progresses through the power stroke, the temperature and pressure eventually decline to a level where reaction rates again become inconsequential. The actual point in the cycle where reaction rates cease to be important will vary from problem to problem. It does seem reasonable to expect that reaction rates will be insignificant by the time the intake valve opens to admit fresh charge to the cylinder, at $\theta = \theta_o^{(+)}$, since this generally occurs quite late in the cycle. Thus the assumption will be made that the volumetric production rates R_λ are identically zero from the time the intake valve opens until the start of combustion.

$$R_\lambda = 0 \qquad \theta_o^{(+)} \leq \theta \leq \theta_0 \tag{III-28}$$

If the flame zone is considered to be the equilibrium state generated from the unburned gas at its pressure and enthalpy, then the equilibrium state will change as the state of the unburned gas changes. This implies that the equilibrium state must be recalculated as combustion proceeds. The effect of a change in enthalpy and pressure on the flame zone temperature can be estimated to first order quite easily. If T_f is the flame zone temperature, then the change in T_f, ΔT_f, produced by a change Δh_2 in the unburned-gas enthalpy and a change Δp_2 in its pressure is, to first order,

$$\Delta T_f = \left(\frac{\partial T_f}{\partial h_f}\right)_{p_f} \Delta h_2 + \left(\frac{\partial T_f}{\partial p_f}\right)_{h_f} \Delta p_2 \tag{III-29}$$

where the derivatives are calculated for the flame zone. The equilibrium state is recalculated whenever $\Delta T_f \geq 20$ K. For $\Delta T_f < 20$ K the flame zone temperature is estimated by equation (III-29) and its composition $n_\lambda^{(f)}$ is estimated from a similar first order approximation.

$$\Delta \ln n_\lambda^{(f)} = \left[\frac{\partial \ln n_\lambda^{(f)}}{\partial \ln T_f}\right]_{p_f} \Delta \ln T_f + \left[\frac{\partial \ln n_\lambda^{(f)}}{\partial \ln p_f}\right]_{T_f} \Delta \ln p_f \qquad \text{(III-30)}$$

The termination of the combustion phase θ^* is determined as the solution of $M_b(\theta^*)/M(\theta_0)=0.9999$ with $M_b(\theta_0)/M(\theta_0)=0.0001$. For $\tau=0$, M_b equals M_f and it is possible to solve for θ^* in closed form for the linear burning function (eq. (I-103)) and the cosine burning function, which is special case of Fourier burning (eq. (I-92)).

$$\theta^* = \begin{cases} \theta_0 + \left(\dfrac{0.9998}{0.9999}\right)(\theta_f - \theta_0) & \text{linear} \\[2ex] \theta_0 + \dfrac{(\theta_f - \theta_0)}{\pi}\cos^{-1}\left(-\dfrac{0.9997}{0.9999}\right) & \text{cosine} \end{cases} \qquad \tau = 0 \qquad \text{(III-31)}$$

The general Fourier burning case is solved for θ^* iteratively in terms of the variable $z=\pi(\theta-\theta_0)/(\theta_f-\theta_0)$.

$$z^{(n+1)} = z^{(n)} + \Delta z^{(n)}$$

$$\Delta z = \begin{cases} \dfrac{2\Delta g}{\dot g + \sqrt{(\dot g)^2 + 2\ddot g\,\Delta g}} & (\dot g)^2 + 2\ddot g\,\Delta g \geq 0 \\[3ex] \dfrac{\Delta g}{\dot g} & (\dot g)^2 + 2\ddot g\,\Delta g < 0 \end{cases} \qquad \text{Fourier, } \tau = 0 \qquad \text{(III-32)}$$

$$g(z) = \sum_{m=0}^{\infty} a_m \cos m\pi z, \qquad \Delta g = \frac{0.9998}{0.9999} - g(z)$$

The initial estimate for θ^* is $\theta_0 + 0.9(\theta_f - \theta_0)$, with convergence to a hundredth of a degree. When $\tau \neq 0$ the assumption is made that $\theta^* \geq \theta_f$ for the linear and Fourier burning. If $\theta^* \geq \theta_f$, then

$$\theta^* = \theta_f + \omega\tau \ln\left\{\left[1 - \frac{M_b(\theta_f)}{M(\theta_0)}\right] \times 10^4\right\} \qquad \frac{M_b(\theta_f)}{M(\theta_0)} \leq 0.9999 \qquad \tau \neq 0 \qquad \text{(III-33)}$$

which applies to linear, cosine, and Fourier burning. It also is valid for Wiebe burning (eq. (I-101)) when $M_b(\theta_f)/M(\theta_0) \leq 0.9999$. When $0.9999 < M_b(\theta_f)/M(\theta_0)$, then

$$\theta^* = \theta_0 + (\theta_f - \theta_0)[\alpha^{-1}\ln(9999)]^{1/\beta} \qquad 0.9999 < \frac{M_b(\theta_f)}{M(\theta_0)} \qquad \text{Wiebe, } \tau \neq 0 \qquad \text{(III-34)}$$

is the appropriate solution for the combustion end point.

Intake and Exhaust Flows

The treatment of intake and exhaust flows within the framework of a cycle simulation is a major complication in the construction of a numerical model. Not only must one contend with points of flow reversals $[\dot M^{(\pm)}=0]$, but also one must locate the points where $M^{(\pm)}$ changes sign. Both kinds of points are a part of the definition of the flow-related functions (I-121) and (I-122). In the general case the points $M^{(\pm)}=0$ and $\dot M^{(\pm)}=0$ can occur in any sequence, and about all one can say in advance with any certainty is that, when the valves close, $M^{(+)}$ will be positive and $M^{(-)}$ will be negative since there is a net mass flow through the engine. To treat the problem with complete generality would require one to estimate, at each step of the calculation, the next occurrence of an

$\dot{M}^{(\pm)}=0$ point and $M^{(\pm)}=0$ point and to proceed on the basis of which occurs first. This becomes particularly vexing during that portion of the cycle where there is valve overlap. To mitigate these difficulties somewhat, it is necessary to limit the generality of $M^{(\pm)}$ by imposing some restrictions. The assumption will be made that, if $M^{(\pm)}$ changes sign, it will do so only once and that will occur shortly after the valve opens. After this sign change in $M^{(\pm)}$ only flow reversals may occur. Of course these restrictions are not enforced at the defined discontinuity in $M^{(+)}$ located at the point where $M^{(+)}$ attains its maximum value $M^{(+)}_{\text{max}}$. The allowed behavior of $M^{(\pm)}$ is sketched in figure 2 and seems to be adequate for the range of behavior normally encountered.

Associated with the calculation of intake and exhaust flows is the task of determining the critical pressure ratio, that is, solving equation (I-115).

$$f\left[(p_2/p_1)_c\right] = \begin{cases} 2\sigma^{(\pm)} - (\gamma_1+1)\left(\dfrac{p_2}{p_1}\right)_c^{(\gamma_1-1)/\gamma_1} + b^{(\pm)}(\gamma_1-1)\left(\dfrac{p_2}{p_1}\right)_c^{(\gamma_1+1)/\gamma_1} = 0 & \gamma_1 \neq 1 \\[2ex] 1 - 2\sigma^{(\pm)} - b^{(\pm)}\left(\dfrac{p_2}{p_1}\right)_c^2 + 2\ln\left(\dfrac{p_2}{p_1}\right)_c = 0 & \gamma_1 = 1 \end{cases} \qquad \text{(III-35)}$$

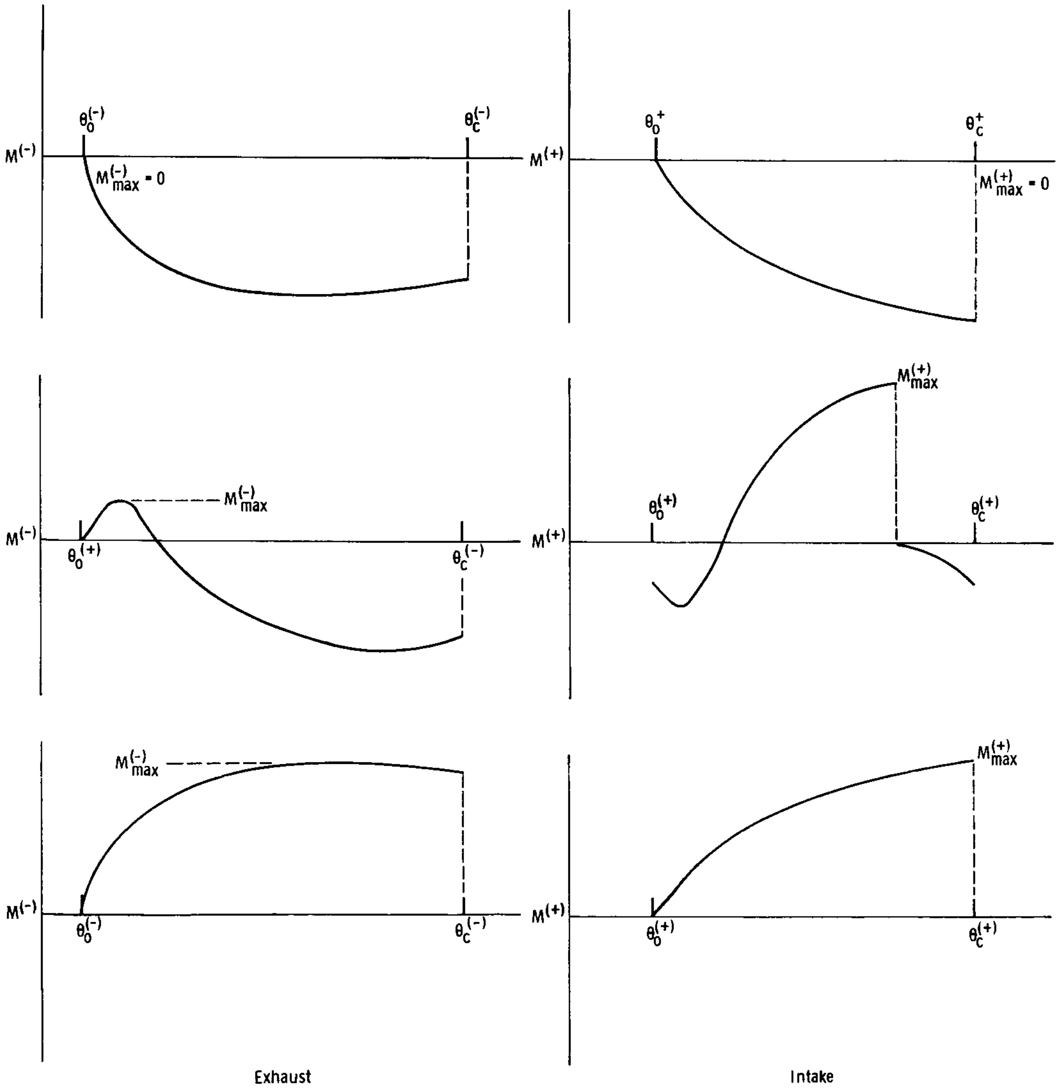


Figure 2. - Permissible intake and exhaust flow behavior.

This can be solved by a Newton-Raphson iteration.

$$x^{(n+1)}=x^{(n)}+\Delta x^{(n)}, \qquad \Delta x=-\frac{f(x)}{\dot{f}(x)} \tag{III-36}$$

Convergence is achieved when $|\Delta x|\leq 10^{-5}$. When the contribution to f from the term involving $b^{(\pm)}$ can be regarded as small, which will generally be true, it is possible to obtain an excellent initial approximation. This can be done by solving the equation with $b^{(\pm)}=0$ and then using this solution to approximate the contribution from the $b^{(\pm)}$ term.

$$\left(\frac{p_2}{p_1}\right)_c^{(0)}=\begin{cases} \left\{\dfrac{2\sigma^{(\pm)}+(\gamma_1-1)b^{(\pm)}\left[2\sigma^{(\pm)}/(\gamma_1+1)\right]^{(\gamma_1+1)/(\gamma_1-1)}}{\gamma_1+1}\right\}^{\gamma_1/(\gamma_1-1)} & \gamma_1\neq 1 \\ \exp\left\{\dfrac{[2\sigma^{(\pm,}-1]+b^{(\pm)}e^{(2\sigma^{(\pm)}-1)}}{2}\right\} & \gamma_1=1 \end{cases} \tag{III-37}$$

The equations for the absolute value of the mass flow rate, (I–110) and (I–112), are nonlinear in $\dot{M}^{(\pm)}$ because the parameters $A^{(\pm)}$, $\sigma^{(\pm)}$, and $b^{(\pm)}$ (eq. (I–117a)) are functions of the Reynolds number (eq. (I–116)), which is itself a function of $|\dot{M}^{(\pm)}|$. Hence the calculation of $|\dot{M}^{(\pm)}|$, which is equivalent to solving

$$F\equiv\begin{cases} |\dot{M}^{(\pm)}|-\dfrac{\rho_1 A^{(\pm)}}{\omega}\sqrt{\dfrac{2p_1\rho_1^{-1}\gamma_1(\gamma_1-1)\left[\sigma^{(\pm)}-(p_2/p_1)^{(\gamma_1-1)/\gamma_1}\right]}{(p_1/p_2)^{2/\gamma_1}-b^{(\pm)}}}=0 & \gamma_1\neq 1 \\ |\dot{M}^{(\pm)}|-\dfrac{\rho_1 A^{(\pm)}}{\omega}\sqrt{\dfrac{2p_1\rho_1^{-1}\left[\sigma^{(\pm)}+\ln(p_1/p_2)\right]}{(p_1/p_2)^2-b^{(\pm)}}}=0 & \gamma_1=1 \end{cases} \tag{III-38}$$

for $|\dot{M}^{(\pm)}|$, must be accomplished with some iterative process. The nonnegativity of $|\dot{M}^{(\pm)}|$ suggests that ln $|\dot{M}^{(\pm)}|$ is an appropriate iteration variable in a Newton-Raphson iteration because this automatically incorporates the nonnegativity constraint on the iteration.

$$\ln|\dot{M}^{(\pm)}|^{(n+1)}=\ln|\dot{M}^{(\pm)}|^{(n)}+\Delta\ln|\dot{M}^{(\pm)}|^{(n)},\qquad \Delta\ln|\dot{M}^{(\pm)}|=-\frac{F}{dF/d\ln|\dot{M}^{(\pm)}|}$$

$$\frac{dF}{d\ln|\dot{M}^{(\pm)}|}=|\dot{M}^{(\pm)}|+\frac{1}{2}[|\dot{M}^{(\pm)}|-F]\left\{\left[\left(\frac{p_1}{p_2}\right)^{2/\gamma_1}-b^{(\pm)}\right]^{-1}\frac{db^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}\right.$$

$$\left.-2\frac{d\ln A^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}\right\}-\frac{1}{2}[|\dot{M}^{(\pm)}|-F]^{-1}\left[\frac{\rho_1 A^{(\pm)}}{\omega}\right]^2\frac{2p_1\rho_1^{-1}}{(p_1/p_2)^{2/\gamma_1}-b^{(\pm)}}\frac{d\sigma^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}$$

(III-39)

$$\frac{d\sigma^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}=\begin{cases}\left(\dfrac{\gamma_1-1}{\gamma_1}\right)\left[E_1^{(\pm)}E_4^{(\pm)}+E_2^{(\pm)}\left(E_3^{(\pm)}+E_4^{(\pm)}\right)(\mathrm{Re}\times 10^{-6})^{E_4^{(\pm)}}\right] & \gamma_1\neq \\[2ex] E_1^{(\pm)}E_4^{(\pm)}+E_2^{(\pm)}\left(E_3^{(\pm)}+E_4^{(\pm)}\right)(\mathrm{Re}\times 10^{-6})^{E_4^{(\pm)}} & \gamma_1=1\end{cases}$$

$$\frac{d\ln A^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}=\frac{A_2^{(\pm)}A_3^{(\pm)}(\mathrm{Re}\times 10^{-6})^{A_3^{(\pm)}}}{A_1+A_2(\mathrm{Re}\times 10^{-6})^{A_3^{(\pm)}}},\qquad \frac{db^{(\pm)}}{d\ln|\dot{M}^{(\pm)}|}=b_2^{(\pm)}b_3^{(\pm)}(\mathrm{Re}\times 10^{-6})^{b_3^{(\pm)}}$$

The change in $|\dot{M}^{(\pm)}|$ per iteration step is limited to about a factor of 10, and the iteration is terminated when $|F|\leq 10^{-4}$.

Integration Methods

The integration methods chosen to solve the systems of first order differential equations (III-1) and (III-2) are those of Theorem III.2 of Chapter II. The vector ℓ is chosen in one of two ways. For those portions of the cycle where $R_\lambda=0$ (eq. (III-28)) the vector is determined by using, from Chapter II, the vectors Tu of table I for $k=1$, weighted as in equation (II-97) to give $\ell_1=1$, and ℓ_0 and V chosen as in equation (II-98). For the other portions of the cycle the vector ℓ is determined by using the vector Tu of table I for $k=0$, also of Chapter II weighted as in equation (II-97) to give $\ell_1=1$. The integration error at each step of the integration is calculated from equations (II-99), (II-106), and (II-107). The norm (eq. II-108)) is obtained by using equation (II-109) with $U^{(k)}$ as the identity matrix, and $E^{(k)}$ is chosen as in equations (II-112), (II-113), and (II-115). The integration equations are solved by a modified Newton-Raphson iteration with no control on the size of the correction. The iteration is deemed to have converged to an adequate solution of the integration equations when any one of three criteria is satisfied. The first of the three tests places a condition on how well the differential equation must be satisfied in the sense of the norm. The iteration is attempting to generate a solution of first order differential equations $\dot{y}-\varphi(y,x)=0$ by determining a vector z_{q+1} whose definition is given in Definition I.2 of Chapter II. Thus

$$\|\dot{y}-\varphi(y,x)\| \leq \epsilon_z = 10^{-2} \tag{III-40}$$

is required to hold. The second criterion is based on the size of the correction $\Delta z_{q+1}^{(n)}$ relative to the current estimate of z_{q+1}, again taken in the sense of the norm.

$$\|\Delta z_{q+1}^{(n)}\| \leq 0.2 \|z_{q+1}^{(n)}+\Delta z_{q+1}^{(n)}\| \tag{III-41}$$

The last criterion is based on how rapidly the iteration is improving the solution to the differential equation. This criterion is effective only after two iterations.

$$\left| \|\dot{y}-\varphi\|^{(n)} - \|\dot{y}-\varphi\|^{(n-1)} \right| \leq 10^{-3} \|\dot{y}-\varphi\|^{(n-1)} \tag{III-42}$$

The order of the integration method and the step size are based on equation (II-104), for which the parameters are

$$\epsilon = 10^{-4}, \quad \gamma_{q-1}=1, \quad \gamma_q = 1.4, \quad \gamma_{q+1}=1 \tag{III-43}$$

and reflect a 40 percent bias against changing order because γ_q is 40 percent larger than either γ_{q-1} or γ_{q+1}.

Equations for First Specialization of Model

Differential Equations and Additional Derivatives

The assumptions associated with the first specialization of the general model effect a considerable simplification in the calculations. These simplifications are of two basic types: those associated with a reduction in numerical details and bookkeeping tasks, and those associated with a simplification of the differential equations. The first type occurs because, effectively, flow reversals have been proscribed, valve overlap has been eliminated, and intake and exhaust flows are confined to smaller crankangle intervals. Flow reversals, if they occur at all, can occur only at the instant of valve opening and serve only to equalize the pressure of the working fluid and the manifold or exhaust pressure. The second type of simplification comes about because of a basic reduction in the complexity of the governing differential equations (I-124), (I-125), and (I-128). Thus, for example, while the equations of the general model still apply from the initiation of combustion to the opening of the exhaust valve, their forms were considerably simplified because in this crankangle interval $\dot{M}^{(\pm)}=0$ and a number of terms in these equations disappeared. Also the differential equation for mass need not be integrated numerically since in the postcombustion part of the cycle the mass in the cylinder remains constant and during combustion the mass of the burned gas is given by $M_1=M_b$.

Finally when the intake or exhaust valve is opened, only a single differential equation requires numerical integration.

Crankangle interval $0 \leq \theta \leq \theta_o^{(+)}$ ***and*** $\pi = \theta_c^{(+)} \leq \theta \leq \theta_0$. – Only one differential equation requires numerical integration for this range of crankangles.

$$\frac{du}{d\theta} = -\frac{p}{\rho}\frac{d\ln V}{d\theta} - \frac{\dot{Q}}{M\omega} \tag{III-44a}$$

The second derivative of u can be approximated as

$$\frac{d^2u}{d\theta^2} = -\frac{p}{M}\left(\frac{d^2V}{d\theta^2} + \frac{d\ln p}{d\theta}\frac{dV}{d\theta}\right) - \frac{\bar{h}A}{M\omega}T\frac{d\ln T}{d\theta} - \frac{\dot{Q}}{M\omega}\frac{d\ln A}{d\theta} \tag{III-44b}$$

by assuming $d\bar{h}/d\theta = 0$. The pressure and temperature derivatives can be expressed exactly, as can the derivative of the area. The rate of change of the heat transfer area with crankangle is obtained by differentiating equation (I-88) and has a form similar to the expression for $dV/d\theta$ (eq. (III-21)).

$$\frac{dA}{d\theta} = 4B^{-1}\frac{dV}{d\theta}$$

$$\frac{d\ln p}{d\theta} = \left(\frac{\partial \ln p}{\partial u}\right)_{\rho,n_\lambda}\frac{du}{d\theta} - \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{u,n_\lambda}\frac{d\ln V}{d\theta} \tag{III-45}$$

$$\frac{d\ln T}{d\theta} = \left(\frac{\partial \ln T}{\partial u}\right)_{\rho,n_\lambda}\frac{du}{d\theta} - \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_{u,n_\lambda}\frac{d\ln V}{d\theta}$$

The pressure and temperature derivative expressions come about by using $dn_\lambda/d\theta = 0$ and $d\ln \rho/d\theta = -d\ln V/d\theta$.

Crankangle interval $\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)} = \pi$. – This crankangle interval corresponds to that part of the cycle where fresh charge is inducted into the cylinder. Here too only one differential equation requires numerical integration, and that equation is chosen as the density equation (I-128).

$$\frac{d\ln \rho}{d\theta} =$$

$$\frac{\left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda}\frac{\dot{Q}}{M\omega}\left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda} + \left\{\left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T} - h^{(0)}\right] - \left(n_\lambda^{(0)} - n_\lambda\right)\left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{T,\rho}\right\}\frac{d\ln V}{d\theta}}{\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{T,n_\lambda} + \left(n_\lambda^{(0)} - n_\lambda\right)\left(\frac{\partial \ln p}{\partial n_\lambda}\right)_{T,\rho} - \left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T} - h^{(0)}\right]}$$

$$\tag{III-46}$$

The second derivative of the density can be approximated by differentiating the first derivative (III-46) and in the differentiation process neglecting the θ dependence of all terms except M and $d\ln V/d\theta$.

$$\frac{d^2\rho}{d\theta^2}=\rho\left[\frac{d^2\ln\rho}{d\theta^2}+\left(\frac{d\ln\rho}{d\theta}\right)^2\right]$$

$$\frac{d^2\ln\rho}{d\theta^2}=$$

$$\frac{-\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\frac{\dot Q}{M\omega}\frac{d\ln M}{d\theta}+\left\{\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T}-h^{(0)}\right]-\left(n_\lambda^{(0)}-n_\lambda\right)\left(\frac{\partial\ln p}{\partial n_\lambda}\right)_{T,\rho}\right\}\frac{d^2\ln V}{d\theta^2}}{\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_\lambda}+\left(n_\lambda^{(0)}-n_\lambda\right)\left(\frac{\partial\ln p}{\partial n_\lambda}\right)_{T,\rho}-\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T}-h^{(0)}\right]}$$

(III-47)

$$\frac{d\ln M}{d\theta}=\frac{\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_\lambda}\frac{d\ln V}{d\theta}+\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\frac{\dot Q}{M\omega}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}}{\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_\lambda}+\left(n_\lambda^{(0)}-n_\lambda\right)\left(\frac{\partial\ln p}{\partial n_\lambda}\right)_{T,\rho}-\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\left(\frac{\partial h}{\partial n_\lambda}\right)_{p,T}-h^{(0)}\right]}$$

$$\frac{d^2\ln V}{d\theta^2}=V^{-1}\frac{d^2V}{d\theta^2}-\left(\frac{d\ln V}{d\theta}\right)^2$$

The third member of this set of equations is just the first member of equation (I-128a). To carry out the integration of equation (III-46), it is also necessary to know the first and second derivatives of the enthalpy because the thermodynamic state in this crankangle interval will be specified by enthalpy and pressure.

$$\frac{dh}{d\theta}=-\frac{\dot Q}{M\omega}+\left(h^{(0)}-h\right)\frac{d\ln M}{d\theta}$$

$$\frac{d^2h}{d\theta^2}=\frac{\dot Q}{M\omega}\left(\frac{d\ln M}{d\theta}-\frac{d\ln A}{d\theta}\right)-\frac{\bar hA}{M\omega}T\frac{d\ln T}{d\theta}+\left(h^{(0)}-h\right)\frac{d^2\ln M}{d\theta^2}-\frac{dh}{d\theta}\frac{d\ln M}{d\theta}$$

$$\frac{d\ln T}{d\theta}=\left(\frac{\partial\ln T}{\partial h}\right)_p\frac{dh}{d\theta}$$

(III-48)

$$\frac{d^2\ln M}{d\theta^2}=\frac{\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_\lambda}\frac{d^2\ln V}{d\theta^2}-\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\left[\frac{\dot Q}{M\omega}\left(\frac{d\ln M}{d\theta}-\frac{d\ln A}{d\theta}\right)-\frac{\bar hA}{M\omega}T\frac{d\ln T}{d\theta}\right]}{\left(\frac{\partial\ln p}{\partial\ln\rho}\right)_{T,n_\lambda}+\left(n_\lambda^{(0)}-n_\lambda\right)\frac{\partial\ln p}{\partial n_\lambda}-\left(\frac{\partial\ln p}{\partial\ln T}\right)_{\rho,n_\lambda}\left(\frac{\partial\ln T}{\partial h}\right)_{p,n_\lambda}\left[n_\lambda^{(0)}\frac{\partial h}{\partial n_\lambda}-h^{(0)}\right]}$$

The calculation of $d^2h/d\theta^2$ assumes $d\bar h/d\theta=0$. The expression for $d^2\ln M/d\theta^2$ is obtained by differentiating the third member of equation (III-47) neglecting all θ dependence except in $d\ln V/d\theta$ and $\dot Q/M\omega$.

Crankangle interval $\theta^*\le\theta\le\theta_o^{(-)}=3\pi$. – The differential equations and their Jacobian are exactly the same as the ones for the noncombustion phase of the general model, equations (III-1) and (III-6), with $\dot M^{(\pm)}=0$ and the equation for mass deleted.

Crankangle interval $3\pi=\theta_o^{(-)}\le\theta\le\theta_c^{(-)}=4\pi$. – The enthalpy differential equation is the only one which requires numerical integration.

$$\frac{dh}{d\theta} = -\frac{\dot{Q}}{M\omega} \tag{III-49}$$

The second derivative of the enthalpy is easily calculated when $d\bar{h}/d\theta = 0$.

$$\frac{d^2h}{d\theta^2} = \frac{\dot{Q}}{M\omega}\left(\frac{d \ln M}{d\theta} - \frac{d \ln A}{d\theta}\right) - \frac{\bar{h}A}{M\omega} T \frac{d \ln T}{d\theta}$$

$$\frac{d \ln M}{d\theta} = \left[\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{T,n_\lambda} \frac{d \ln V}{d\theta} + \left(\frac{\partial \ln p}{\partial \ln T}\right)_{\rho,n_\lambda} \left(\frac{\partial \ln T}{\partial h}\right)_p \frac{\dot{Q}}{M\omega}\right] \Bigg/ \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{T,n_\lambda} \tag{III-50}$$

$$\frac{d \ln T}{d\theta} = \left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda} \left(\frac{dh}{d\theta}\right)$$

Crankangle interval $\theta_0 \leq \theta \leq \theta^*$. – The differential equations and their Jacobian are precisely the ones for the combustion phase of the general model (eqs. (III-2) and (III-11)) with $\dot{M}_1^{(-)} = 0$ and the equation for burned mass M_1 deleted.

Calculations at Pressure Discontinuities

In this model of the internal combustion engine a pressure discontinuity will occur at $\theta = 0$ if and only if $p(0) < p_m$, and one will occur at $\theta = 3\pi$ if and only if $p(3\pi) \neq p_e$. If $p(3\pi) > p_e$, then a simple expansion to p_e by one of the processes (I-118) will determine the density and hence the mass which must be removed from the cylinder so that the pressure will equal p_e. If $p(0) < p_m$ or $p(3\pi) < p_e$, then the pressures are equalized (to p_m or p_e) in two separate stages. First, the cylinder contents are compressed (to p_m or p_e) by one of the two processes (I-118), and this is followed by mass addition at constant pressure. At $\theta = 0$ the added mass is fresh charge, while at $\theta = 3\pi$ it is the composite exhaust gas from the preceding cycle. The amount of mass to be added must be calculated iteratively, and since the composition, enthalpy, and mass are given in terms of E_m by equations (I-126) and (I-129), this implies the iterative calculation of E_m.

Consider first the situation at $\theta = \theta_o^{(+)} = 0$. Since the mass addition takes place at constant pressure, it follows from the pair of functions (I-127) that to first order

$$\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_T \Delta \ln \rho + \left(\frac{\partial \ln p}{\partial \ln T}\right)_\rho \Delta \ln T + \frac{\partial \ln p}{\partial n_\lambda} \Delta n_\lambda = 0$$

$$\left(\frac{\partial h}{\partial \ln T}\right)_p \Delta \ln T + \frac{\partial h}{\partial n_\lambda} \Delta n_\lambda = \Delta h \tag{III-51}$$

must be satisfied during mass addition. Suppose $\Delta \ln \rho$, Δh and Δn_λ are interpreted as the difference between the values calculated from equations (I-126) and (I-129) and estimates for ρ, h, and n_λ.

$$\Delta \ln \rho = \frac{\Delta\rho}{\rho} = \frac{\rho[\theta_o^{(+)}](1 + E_m) - \rho}{\rho}$$

$$\Delta h = \frac{h[\theta_o^{(+)}] + E_m h^{(0)}}{1 + E_m} - h = \frac{h[\theta_o^{(+)}] - h^{(0)} + (1 + E_m)[h^{(0)} - h]}{1 + E_m} \tag{III-52}$$

$$\Delta n_\lambda = \frac{n_\lambda(\theta_o^{(+)}) - n_\lambda^{(0)} + (1 + E_m)[n_\lambda^{(0)} - n_\lambda]}{1 + E_m}$$

The values at $\theta_o^{(+)}$ in these equations are the values after compression to p_m. If $\Delta \ln T$ is eliminated between the two members of equation (III-51), followed by substitution from equation (III-52), then the resulting equation can be written as a quadratic in $(1+E_m)$ whose solution will yield an improved estimate for E_m. When the values of $(\partial \ln p/\partial \ln T)_\rho$, $(\partial \ln p/\partial \ln \rho)_T$, $\partial \ln p/\partial n_\lambda$, and $\partial h/\partial n_\lambda$ are substituted into the quadratic, we find

$$\tilde{a}(1+E_m)^2+\tilde{b}(1+E_m)+\tilde{c}=0$$

$$\tilde{a}=1$$

$$\tilde{b}=\frac{-\rho}{\rho\left[\theta_o^{(+)}\right]}\left\{1-\left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda}\left[h^{(0)}-{}^*H^\lambda n_\lambda^{(0)}\right]-\frac{\sum\limits_\lambda n_\lambda^{(0)}-\sum\limits_\lambda n_\lambda}{\sum\limits_\tau n_\tau}\right\} \tag{III-53}$$

$$\tilde{c}=\frac{\rho}{\rho\left[\theta_o^{(+)}\right]}\left\{\left(\frac{\partial \ln T}{\partial h}\right)_{p,n_\lambda}\left(h\left[\theta_o^{(+)}\right]-h^{(0)}-{}^*H^\lambda\left\{n_\lambda\left[\theta_o^{(+)}\right]-n_\lambda^{(0)}\right\}\right)\right.$$
$$\left.+\frac{\sum\limits_\lambda n_\lambda\left(\theta_o^{(+)}\right)-\sum\limits_\lambda n_\lambda^{(0)}}{\sum\limits_\tau n_\tau}\right\}$$

and then

$$1+E_m=\frac{-\tilde{b}\left(1+\sqrt{1-4\tilde{c}/\tilde{b}^2}\right)}{2} \tag{III-54}$$

is the appropriate root. The initial estimate for E_m is obtained by assuming that the cylinder volume available because of compression to p_m is filled with fresh charge. If $'\rho\left(\theta_o^{(+)}\right)$ is the density prior to compression then

$$E_m^{(0)}=\frac{\rho^{(0)}}{\rho\left[\theta_o^{(+)}\right]}\left\{\frac{\rho\left[\theta_o^{(+)}\right]}{'\rho\left[\theta_o^{(+)}\right]}-1\right\} \tag{III-55}$$

provides a good estimate. It is assumed that the calculation has converged when

$$\left|\frac{E_m^{(n+1)}-E_m^{(n)}}{E_m^{(n+1)}}\right|<0.5\times 10^{-4} \tag{III-56}$$

The corresponding calculation for the exhaust, while still an iterative calculation of the relative mass charge, is carried out somewhat differently. Here the calculation focuses on φ, the ratio of the density calculated from the equation of state (I-132) to that calculated from the mass and volume. Equations analogous to (I-126) and (I-129) apply here except that $\theta_o^{(+)}$ is replaced by $\theta_o^{(-)}$, $h^{(0)}$ becomes $h^{(e)}$, and $n_\lambda^{(0)}$ becomes $n_\lambda^{(e)}$.

$$\varphi\equiv\frac{p_e}{RT\sum\limits_\lambda n_\lambda}\left\{(1+E_m)\,'\rho\left[\theta_o^{(-)}\right]\right\}^{-1},\qquad h=\frac{h\left[\theta_o^{(-)}\right]+E_m h^{(e)}}{1+E_m}$$
$$n_\lambda=\frac{n_\lambda\left[\theta_o^{(-)}\right]+E_m n_\lambda^{(e)}}{1+E_m},\qquad E_m=\frac{M-{}'M\left[\theta_o^{(-)}\right]}{'M\left[\theta_o^{(-)}\right]} \tag{III-57}$$

In these equations $'\rho[\theta_o^{(-)}]$ and $'M[\theta_o^{(-)}]$ are values prior to compression to p_e. The unprimed quantities at $\theta_o^{(-)}$ are the values following compression to p_e. When the calculation converges, φ will have the value unity and a Newton-Raphson iteration for ln E_m takes the form

$$\ln \varphi + \frac{d \ln \varphi}{d \ln E_m} \Delta \ln E_m = 0 \qquad \text{(III-58)}$$

where $d \ln \varphi / d \ln E_m$ must still be calculated.

$$\frac{d \ln \varphi}{d \ln E_m} = - \frac{d \ln T}{d \ln E_m} - \left(\sum_{\tau} n_{\tau} \right)^{-1} \sum_{\lambda} \frac{dn_{\lambda}}{d \ln E_m} - \frac{E_m}{1 + E_m} \qquad \text{(III-59)}$$

The contribution of the composition derivative is easily evaluated by a differentiation of the composition equation in (III-57).

$$\left(\sum_{\tau} n_{\tau} \right)^{-1} \sum_{\lambda} \frac{dn_{\lambda}}{d \ln E_m} = \frac{\left(\left\{ \sum_{\lambda} n_{\lambda}[\theta_o^{(-)}] \right\}^{-1} - \left[\sum_{\lambda} n_{\lambda}^{(e)} \right]^{-1} \right) E_m \Big/ (1 + E_m)^2}{\left(\left[\sum_{\lambda} n_{\lambda}^{(e)} \right]^{-1} + E_m \left\{ \sum_{\lambda} n_{\lambda}[\theta_o^{(-)}] \right\}^{-1} \right) \Big/ (1 + E_m)} \qquad \text{(III-60)}$$

The temperature derivative must be evaluated by a differentiation of the enthalpy equation in (III-57). Because the enthalpy is linear in composition (eq. (I-131)), the enthalpy may be written as

$$h = {}^*H^{\lambda}(T) n_{\lambda} = \frac{{}^*H^{\lambda}(T) n_{\lambda}[\theta_o^{(-)}] + E_m {}^*H^{\lambda}(T) n_{\lambda}^{(e)}}{1 + E_m} \qquad \text{(III-61)}$$

by a substitution of the composition equation from (III-57), and this may be regarded as a function of T and E_m. If the expression (III-61) is used on the left side of the enthalpy equation (III-57) and the resulting equation is differentiated with respect to ln E_m, then this produces an expression for $d \ln T / d \ln E_m$.

$$\frac{\partial h}{\partial \ln T} \frac{d \ln T}{d \ln E_m} = \frac{\left\{ \left[h^{(e)} - {}^*H^{\lambda}(T) n_{\lambda}^{(e)} \right] - \left[h\left(\theta_o^{(-)}\right) - {}^*H^{\lambda}(T) n_{\lambda}\left(\theta_o^{(-)}\right) \right] \right\} E_m}{(1 + E_m)^2} \qquad \text{(III-62)}$$

The iteration on E_m is continued until the condition

$$|\varphi - 1| \leq 10^{-4} \qquad \text{(III-63)}$$

is satisfied. An initial estimate for E_m is obtained by setting φ to unity and assuming that ${}^*H^{\lambda}$ is linear in temperature. The linearity of ${}^*H^{\lambda}$ implies that

$${}^*H^{\lambda}(T) n_{\lambda}\left(\theta_o^{(-)}\right) \cong h\left(\theta_o^{(-)}\right) + \left\{ T - T[\theta_o^{(-)}] \right\} \left({}^*C^{\lambda} \left\{ T[\theta_o^{(-)}] \right\} n_{\lambda}[\theta_o^{(-)}] + R \sum_{\lambda} n_{\lambda}[\theta_o^{(-)}] \right)$$

$${}^*H^{\lambda}(T) n_{\lambda}^{(e)} \cong h^{(e)} + (T - T_e) \left[{}^*C^{\lambda}(T_e) n_{\lambda}^{(e)} + R \sum_{\lambda} n_{\lambda}^{(e)} \right]$$

This assumption converts the enthalpy expression (III-61) into an expression linear in temperature and, when used on the left side of the enthalpy equation in (III-57), produces an equation linear in T whose solution for T can be substituted into $\varphi = 1$ to produce a quadratic equation for $E_m^{(0)}$.

$$\tilde{a}[E_m^{(0)}]^2 + \tilde{b}E_m^{(0)} - \tilde{c} = 0, \qquad \tilde{a} = 1/2$$

$$2\tilde{b} = \left\{ \frac{\sum_\lambda n_\lambda[\theta_o^{(-)}]}{\sum_\tau n_\tau^{(e)}} \right\} \left\{ 1 - \frac{p_e}{{}'\rho[\theta_o^{(-)}]RT_e \sum_\lambda n_\lambda(\theta_o^{(-)})} \right\} + \frac{T[\theta_o^{(-)}]c_p[T(\theta_o^{(-)})]}{T_e c_p(T_e)}$$

$$2\tilde{c} = \left[\frac{p_e}{{}'\rho(\theta_o^{(-)})RT(\theta_o^{(-)})\sum_\lambda n_\lambda(\theta_o^{(-)})} - 1 \right] \frac{T(\theta_o^{(-)})c_p[T(\theta_o^{(-)})]\sum_\lambda n_\lambda(\theta_o^{(-)})}{T_e c_p(T_e)\sum_\tau n_\tau^{(e)}} \qquad \text{(III-64)}$$

$$c_p(T_e) \equiv {}^*C^\lambda(T_e)n_\lambda^{(e)} + R\sum_\lambda n_\lambda^{(e)}$$

$$c_p\left\{T[\theta_o^{(-)}]\right\} \equiv {}^*C^\lambda\left\{T[\theta_o^{(-)}]\right\}n_\lambda(\theta_o^{(-)}) + R\sum_\lambda n_\lambda(\theta_o^{(-)})$$

Except for ${}'\rho[\theta_o^{(-)}]$ all values at $\theta_o^{(-)}$ in these equations are those after compression to p_e; ${}'\rho[\theta_o^{(-)}]$ is the density before compression. The initial estimate $E_m^{(0)}$ is the root

$$E_m^{(0)} = \sqrt{\tilde{b}^2 + 2\tilde{c}} - \tilde{b} \qquad \text{(III-65)}$$

Quadrature

Just as for the general model, it is necessary to evaluate the mass content of the cylinder, the work, and the heat transfer for the first specialization of the general model. The calculations are somewhat simpler here because the model itself is a little bit simpler. For example, the mass in the cylinder can be calculated without a quadrature formula. In this model the mass changes only in the intervals $\theta_o^{(+)} \le \theta \le \theta_c^{(+)}$ and $\theta_o^{(-)} \le \theta \le \theta_c^{(-)}$. In the first of these intervals the density is evaluated by integration of equation (III-46), and consequently the mass can be calculated directly as a product of the density and the cylinder volume. During the second of these intervals it is the enthalpy which is calculated. But since the pressure is constant in this interval, the enthalpy and the pressure define the thermodynamic state completely and thus enable the direct calculation of the density. Thus here too the mass can be calculated as a product of the density and volume.

On the other hand, cycle work must still be evaluated by a quadrature over most of the cycle. Over the intervals $\theta_o^{(+)} \le \theta \le \theta_c^{(+)}$ and $\theta_o^{(-)} \le \theta \le \theta_c^{(-)}$, where the mass is changing, the pressure is constant. Consequently the work increment can be calculated as the product of the pressure and a volume increment, and no quadrature formula is needed. Over the other portions of the cycle the work increment is evaluated with the quadrature formula (III-19) in conjunction with equation (III-20). Over the combustion and postcombustion intervals, $\theta_0 \le \theta \le \theta^*$ and $\theta^* \le \theta \le \theta_o^{(-)}$, where chemical kinetics plays a role, the terms in equation (III-20) are calculated as given in equation (III-21). Over the balance of the cycle, $0 \le \theta \le \theta_o^{(+)}$ and $\theta_c^{(+)} \le \theta \le \theta_0$, the last member of equation (III-21) is replaced by the second member of equation (III-45) in calculating the rate of change of pressure with crankangle.

The quadrature for heat transfer is carried out in one of two ways. For the constant-pressure portions of the cycle, $\theta_o^{(+)} \le \theta \le \theta_c^{(+)}$ and $\theta_o^{(-)} \le \theta \le \theta_c^{(-)}$, the heat transfer increment is calculated with adequate accuracy by equation (III-19) with $f = \dot{Q}/\omega$, and this is supplemented with the assumption $\dot{f}_1 = \dot{f}_2$. For the balance of the cycle the heat transfer increment is calculated from an exact formula which can be derived easily from equations (I-124) and (I-125) in conjunction with the first member of equation (I-75).

$$\int \frac{\dot{Q}}{\omega}\, d\theta = -\int p \frac{dV}{d\theta}\, d\theta - \int d(Mu) \qquad \text{if } \frac{dM}{d\theta} = 0 \tag{III-66}$$

The first integral on the right is of course the work integral; the second integral is the change in internal energy for the contents of the cylinder.

Estimation of $\theta_o^{(+)}$ When $p_m < p_e$

If $p(0) = p_e > p_m$, then the intake valve opening is delayed until the pressure has been reduced to p_m by piston motion. The determination of the crankangle where this will occur necessitates an extrapolation of the pressure. The extrapolation formula will be based on equations (III-12) and (III-13) with $f = \ln p$. We have found that quadratic extrapolation is adequate, and the parameter d in equation (III-12) is set to zero. In the notation of equations (III-12) and (III-13) and figure 1 the remaining parameters are

$$a = f_1 = \ln p_1, \qquad b = \dot{f}_1, \qquad c = \frac{\dot{f}_1 - \dot{f}_2}{2h}, \qquad d = 0 \tag{III-67}$$

and should the point θ_2 be unavailable, as would be the case at $\theta = 0$, c is also set to zero. To estimate $\theta_o^{(+)}$, it is only necessary to set $p = p_m$ in the extrapolation formula and to determine the correct root of the quadratic.

$$\theta_o^{(+)} - \theta_1 \cong \frac{2 \ln(p_m/p_1)}{b - \sqrt{b^2 + 4c \ln(p_m/p_1)}} \tag{III-68}$$

The calculation of $\dot{f} = d \ln p/d\theta$ is carried out with the second member of equation (III-45).

Integration Methods

The integration methods are of two types. Where chemical kinetics is a factor, that is, from the initiation of combustion and through the postcombustion phase up to exhaust valve opening, the integration methods are precisely those described for the comparable crankangle interval of the general model. For other portions of the cycle, where only the differential equation requires numerical integration, the method is the Euler method. This method, as pointed out in Chapter II, is the simplest linear, multistep method of Adams' type and is a one-step method. If the differential equation is

$$\frac{dy}{d\theta} = \varphi(y, \theta) \tag{III-69}$$

then, in the notation of figure 1, the Euler method is

$$y_1 = y_2 + \frac{h[\varphi(y_1, \theta_1) + \varphi(y_2, \theta_2)]}{2} \tag{III-70}$$

which is to be solved for y_1. The initial estimate $y_1^{(0)}$ of y_1 is calculated from a Taylor expansion truncated after the second derivative.

$$y_1^{(0)} = y_2 + h\dot{y}_2 + \frac{h^2 \ddot{y}_2}{2} \tag{III-71}$$

Subsequent estimates are calculated iteratively.

$$y_1^{(n+1)} = y_2 + \frac{h\left\{\varphi\left[y_1^{(n)}, \theta_1\right] + \varphi(y_2, \theta_2)\right\}}{2} \tag{III-72}$$

Experience has shown that $y_1^{(1)}$ represents an adequate estimate for y_1 under these circumstances.

The solution of the Euler integration equation (III-70) involves the purely thermodynamic calculation of the state of the working fluid. For crankangle intervals $\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)} = \pi$ and $3\pi = \theta_o^{(-)} \leq \theta \leq \theta_c^{(-)} = 4\pi$, where the pressure remains constant, the thermodynamic state is specified by the enthalpy and the pressure. Elsewhere it is defined by the internal energy and the specific volume ρ^{-1}. Thus, even though only one equation is being integrated, the calculation requires the estimation of two variables. For the interval $\theta_o^{(-)} \leq \theta \leq \theta_c^{(-)}$ this is no problem because the pressure is known to be p_e and the enthalpy can be calculated from the differential equation being integrated. During the interval $\theta_o^{(+)} \leq \theta \leq \theta_c^{(+)}$ the pressure is now p_m but the differential equation determines the evolution of the density and not the enthalpy. But from the density one knows the mass and, through the last member of equation (I-126), the value of E_m. But this estimate of E_m then produces an estimate of the enthalpy by means of equation (I-129). In the remaining intervals the differential equation determines the internal energy. The specification of the state is completed simply by calculating the specific volume from the known, and constant, mass and the known volume available to the working fluid.

The only matter still requiring consideration is the selection of a step size. The Euler method is a one-step method, and the step size is permitted to change at each step. For those portions of the cycle where the thermodynamic state is defined by the internal energy and specific volume, the step size is defined by specifying a maximum change in internal energy during the step. The step is constrained to produce no more than a 1 percent change in internal energy and is further restricted by the condition $\pi/90 \leq h \leq \pi/18$. In the notation of figure 1, using $\bar{h}$ as the estimated step size and h as the actual step size, we have

$$|u_1 - u_2| = 0.01\,|u_2|, \qquad \frac{u_1 - u_2}{\dot{u}_2} = \bar{h}\left(1 + \frac{\bar{h}\ddot{u}_2}{2\dot{u}_2}\right), \qquad h = \max\left\{\frac{\pi}{90}, \min\left\{\bar{h}, \frac{\pi}{18}\right\}\right\} \tag{III-73}$$

as the equations determining the step size. A careful examination of the quadratic for $\bar{h}$, given as the second member of equation (III-73), discloses that the solution for $\bar{h}$ has one of two forms depending on conditions.

$$\bar{h} = \begin{cases} \dfrac{0.02\,|u_2/\dot{u}_2|}{1 + \sqrt{1 + 0.02\,|u_2/\dot{u}_2|\ddot{u}_2/\dot{u}_2}} & \dfrac{\ddot{u}_2}{\dot{u}_2} \geq 0 \text{ or } \left(\dfrac{\ddot{u}_2}{\dot{u}_2} < 0 \quad \text{and} \quad 0.01\left|\dfrac{u_2}{\dot{u}_2}\right| \leq -\dfrac{\dot{u}_2}{2\ddot{u}_2}\right) \\[2ex] \dfrac{-\left(1 + \sqrt{1 - 0.02\,|u_2/\dot{u}_2|\ddot{u}_2/\dot{u}_2}\right)}{\ddot{u}_2/\dot{u}_2} & \dfrac{\ddot{u}_2}{\dot{u}_2} < 0 \quad \text{and} \quad -\dfrac{\dot{u}_2}{2\ddot{u}_2} < 0.01\left|\dfrac{u_2}{\dot{u}_2}\right| \end{cases} \tag{III-74}$$

For those portions of the cycle where the thermodynamic state is defined by the enthalpy and the pressure, the step size is determined in exactly the same way except that the internal energy is replaced by the enthalpy.

Equations for Second Specialization of Model

Differential Equations

This cycle calculation is identical to the first specialization in all respects except for the combustion and postcombustion phases of the cycle. Here chemical equilibrium replaces the chemical kinetics of the first specialization and produces a dramatic reduction in the number of differential equations to be integrated.

Crankangle interval $\theta^* \leq \theta \leq \theta_o^{(-)} = 3\pi$. – In this interval the sole surviving equation from (I-124) is the one for the internal energy and the applicable equations are exactly the same as those given in difference is that now the composition is assumed to be in chemical equilibrium. Consequently the last two members of equation (III-45) must be reinterpreted.

$$\frac{d\ln p}{d\theta} = \left(\frac{\partial \ln p}{\partial u}\right)_\rho \frac{du}{d\theta} - \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_u \frac{d\ln V}{d\theta}$$

$$\frac{d\ln T}{d\theta} = \left(\frac{\partial \ln T}{\partial u}\right)_\rho \frac{du}{d\theta} - \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_u \frac{d\ln V}{d\theta} \tag{III-75}$$

Crankangle interval $\theta_0 \leq \theta \leq \theta^*$. – Here the surviving equations from (I-125) are the two differential equations for the internal energies of the burned and unburned gases. Taking account of the fact that the unburned-gas composition is unchanging while the burned-gas composition is in chemical equilibrium permits the conversion of the internal energy equations into equations for the temperatures.

$$\frac{dT_1}{d\theta} = -\left[\left(\frac{\partial u_1}{\partial T_1}\right)_{\rho_1}\right]^{-1}\left[\frac{p_1}{\rho_1}\frac{(\partial \ln \rho_1/\partial \ln T_1)_{p_1}}{(\partial \ln \rho_1/\partial \ln p_1)_{T_1}}\frac{d\ln \rho_1}{d\theta} + \frac{\dot{Q}_1}{M_1\omega} - (h_2 - h_1)\frac{d\ln M_1}{d\theta}\right]$$

$$\frac{dT_2}{d\theta} = -\left[\left(\frac{\partial u_2}{\partial T_2}\right)_{\rho_2, n_\lambda^{(2)}}\right]^{-1}\left[\frac{p_2}{\rho_2}\frac{(\partial \ln \rho_2/\partial \ln T_2)_{p_2, n_\lambda^{(2)}}}{(\partial \ln \rho_2/\partial \ln p_2)_{T_2, n_\lambda^{(2)}}}\frac{d\ln \rho_2}{d\theta} + \frac{\dot{Q}_2}{M_2\omega}\right] \tag{III-76}$$

The equation corresponding to equation (III-3a) in the pair of equations used to evaluate $d\ln V_1/d\theta$ and $d\ln V_2/d\theta$ (eqs. (I-78), (I-82)) also simplifies considerably because $\dot{M}_1^{(-)} = 0$ and because of equilibrium chemistry.

$$-\gamma_1\frac{d\ln V_1}{d\theta} + \gamma_2\frac{d\ln V_2}{d\theta} = \gamma_2\frac{d\ln M_2}{d\theta} - \frac{\dot{Q}_2}{M_2\omega}\left(\frac{\partial \ln p_2}{\partial u_2}\right)_{\rho_2, n_\lambda^{(2)}} - \gamma_1\frac{d\ln M_1}{d\theta}$$

$$+\left[\frac{\dot{Q}_1}{M_1\omega} - (h_2 - h_1)\frac{d\ln M_1}{d\theta}\right]\left(\frac{\partial \ln p_1}{\partial u_1}\right)_{\rho_1} \tag{III-77}$$

Extrapolation

To carry through the combustion calculations, it is necessary to be able to extrapolate a number of properties. These extrapolations will always be calculated with the polynomial (III-12), whose coefficients are given by equation (I-14). The only differences are in how the polynomial is used and in the actual evaluation of the coefficients.

$$f(\theta) = a + bh\left(\frac{\Delta\theta}{h}\right) + ch^2\left(\frac{\Delta\theta}{h}\right)^2 + dh^3\left(\frac{\Delta\theta}{h}\right)^3, \quad a = f_1, \quad bh = \dot{f}_1 h$$

$$dh^3 = 2\left[f_2 - f_1 + \frac{(\dot{f}_1 + \dot{f}_2)h}{2}\right], \quad ch^2 = f_2 - f_1 + \dot{f}_1 h + dh^3 \tag{III-78}$$

The notation in equation (III-78) is that shown in figure 1. This form of the extrapolating polynomial facilitates setting *d* to zero when desired and avoids divisions by *h* during coefficient evaluation.

Integration Methods

Where this model of the internal combustion engine cycle coincides with the first specialization of the general model, the integration techniques are those used with that model. So it is only necessary to describe the methods used for the combustion and the postcombustion portions of the cycle. The differential equations for these parts of the cycle are also integrated by Euler's method (eq. (III-70)). Of course the y and φ in equation (III-70) are both to be interpreted as two component vectors during combustion because a pair of differential equations is being integrated. During the postcombustion part of the cycle ($\theta^* \le \theta \le 3\pi$) it is the internal energy which is being integrated, and the thermodynamic state of the working fluid is defined by the internal energy and the specific volume. It differs from the other portions of the cycle, where the state is given in terms of these variables only because the chemistry here corresponds to thermodynamic equilibrium. As a result the integration techniques for this portion of the cycle are identical to the methods used for $0 \le \theta \le \theta_o^{(+)}$ and $\pi = \theta_c^{(+)} \le \theta \le \theta_0$, except that the last two members of equation (III-45) are replaced by equation (III-75) in the calculation of the pressure and temperature derivatives.

During combustion the state of the working fluid is presumed to be specified by temperature and specific volume, that is, by T_1,ρ_1^{-1} and T_2,ρ_2^{-1}. The extrapolation of these variables to obtain initial estimates for the solution by Euler's method is accomplished with the polynomial (III-78). Clearly since the temperatures satisfy the equations of Euler's integration method, the cubic coefficient d for temperature must be set to zero. The iterative solution of equation (III-70) is obtained by the iteration process

$$y_1^{(n+1)} = y_1^{(n)} + \lambda^{(n)}\Delta y_1^{(n)}, \qquad \Delta y_1^{(n)} = h\left[\varphi\left(y_1^{(n)},\theta\right) - \varphi\left(y_1^{(n-1)},\theta\right)\right]$$

$$\lambda^{(n)} = \frac{3(n+1)^2}{1+3(n+1)^2} \tag{III-79}$$

where $\lambda^{(n)}$ is an empirical parameter used to control the iteration step size. The vector y in equation (III-79), as mentioned before, stands for the burned- and unburned-gas temperatures T_1 and T_2. Each iteration for the temperatures contains within it a subiteration on the specific volumes. Thus for a given estimate of the temperatures there is an iteration on the specific volumes based on the pair of equations (I-83). This pair of equations can be written in the form

$$\rho_1^{-1} = \frac{V}{M_1 + M_2\rho_1/\rho_2}, \qquad \rho_2^{-1} = \rho_1^{-1}\left(\frac{\rho_1}{\rho_2}\right)$$

and when the density ratio is replaced by its equivalent, using tne equation of state with $p_1 = p_2$, it leads to

$$\left(\rho_1^{-1}\right)^{(m+1)} = \frac{V}{M_1 + M_2T_2\left(\sum_\lambda n_\lambda^{(1)}\right)^{(m)} \Big/ T_1\sum_\lambda n_\lambda^{(2)}}$$

$$\left(\rho_2^{-1}\right)^{(m+1)} = \frac{\left(\rho_1^{-1}\right)^{(m)} T_2 \sum_\lambda n_\lambda^{(2)}}{T_1\left(\sum_\lambda n_\lambda^{(1)}\right)^{(m)}} \tag{III-80}$$

as the iteration for specific volume. A maximum of six iterations is permitted for each type of iteration. The convergence criteria are

$$\left|\left[\left(\rho_1^{-1}\right)^{(m+1)} - \left(\rho_1^{-1}\right)^{(m)}\right] \Big/ \left(\rho_1^{-1}\right)^{(m)}\right| \leq 0.002$$

$$\left|T_1^{(n+1)} - T_1^{(n)}\right| \leq 0.1$$

$$\left|T_2^{(n+1)} - T_2^{(n)}\right| \leq 0.1 \qquad \text{(III-81)}$$

$$\left|p_1^{(n)} - p_2^{(n)}\right| \leq 0.005$$

and if these are not satisfied within the allowed number of iterations, the integration step size is halved and the calculation is then repeated.

Several factors go into the determination of the integration step size during combustion. For the initial step it is arbitrarily set to

$$h_{\text{initial}} = \frac{(\theta_f - \theta_0)}{500} \qquad \text{(III-82)}$$

and thereafter it is calculated, on the basis of the progress of combustion, taking into account the rates of change of pressure and burned-gas internal energy. To formulate an expression for the computation of step size, consider a function $f(\theta)$ with a Taylor expansion in the vicinity of θ_1 for which $f^{(1)}(\theta_1) = f_1^{(1)} \neq 0$.

$$f(\theta_1 + \bar{h}) = \sum_{n=0}^{\infty} \frac{\bar{h}^n f_1^{(n)}}{n!}$$

The contribution of higher derivatives to the function f, relative to the first derivative contribution, may be expressed as the expansion

$$F(\theta_1 + \bar{h}) \equiv \frac{f[\theta_1 + \bar{h}] - f_1^{(0)} - \bar{h} f_1^{(1)}}{\bar{h} f_1^{(1)}} = \sum_{n=1}^{\infty} \frac{\bar{h}^n F_n}{n!}$$

$$F_n \equiv \frac{f_1^{(n+1)}}{(n+1) f_1^{(1)}} \qquad f_1^{(1)} \neq 0 \qquad \text{(III-83)}$$

A value of $\bar{h}$ associated with the function f, $\bar{h}_f$, can be defined by assigning a value, R_f, to $|F|$ and truncating its expansion with the second order term. This yields a quadratic equation for $\bar{h}_f$.

$$F(\bar{h}) \equiv \bar{h} F_1 + \frac{\bar{h}^2 F_2}{2}$$

$$\left|F(\bar{h}_f)\right| = R_f \qquad \text{(III-84)}$$

The form of the solution to this quadratic equation for $\bar{h}_f$ depends on the relationship of F_1 and F_2.

$$\bar{h}_f = \begin{cases} -\dfrac{F_1}{F_2} + \left[(F_1/F_2)^2 + 2R_f/|F_2|\right]^{1/2} & \operatorname{sgn}(F_1) = -\operatorname{sgn}(F_2) \text{ and } 2R_f|F_2| > F_1^2 \\ 2R_f/|F_1|\left\{1 + \left[1 + R_f F_1^{-2}|F_2| \operatorname{sgn}(F_1F_2)\right]^{1/2}\right\} & \text{otherwise} \end{cases} \tag{III-85}$$

Should the first derivative vanish, one could perform the same kind of analysis but now looking at the contributions of higher derivatives relative to the second derivative. This produces a quadratic equation with a form identical to equation (III-84) but with slightly altered definitions of F_n.

$$F_n = \frac{2f_1^{(n+2)}}{(n+1)(n+2)f_1^{(2)}} \qquad f_1^{(1)} = 0, f_1^{(2)} \neq 0 \tag{III-86}$$

With f chosen as the pressure during combustion

$$R_p = 1/2, \qquad |F_1| = \max\left\{ \left| \frac{(\dot{p}_1 - \dot{p}_2)}{(\dot{p}_1 + \dot{p}_2)h} \right|, 0.02 \right\}, \qquad F_2 = 0 \tag{III-87}$$

where, in the calculation of F_1, the second derivative of the pressure has been approximated as a difference of first derivatives divided by the step size and the first derivative has been replaced by the mean of two first derivatives. For f chosen as the internal energy of the burned gas the calculation of F_1 and F_2 is based on the extrapolation formula (III-78) applied to u_1. The coefficients of this extrapolation formula are used as estimates of the derivatives. The F_1 and F_2 are calculated either as in equation (III-83) or as in equation (III-86) depending on the size of $\dot{u}_1$ relative to $\ddot{u}_1$.

$$R_{u_1} = 1/2$$

$$F_1 = \frac{c}{b}, \; F_2 = \frac{2d}{b} \qquad |\dot{u}_1| \geq 1/2 \text{ or } |\dot{u}_1| \geq \frac{|\ddot{u}_1|}{200} \tag{III-88}$$

$$F_1 = \frac{d}{c}, \; F_2 = 0 \qquad \text{otherwise}$$

The step size is then chosen by the prescription

$$h = \max\left\{ \frac{\pi}{900}, \min\left[\frac{\pi}{36}, \frac{10}{|\dot{u}_1|}, \bar{h}_p, \bar{h}_{u_1} \right] \right\} \tag{III-89}$$

although if $M_1(\theta + h)/M_1(\theta) \geq 3$, the step size is halved before use.

Equations for Third Specialization of Model

There are no differential equations which require numerical integration in this thermodynamic model, and all computations can be performed directly without iteration except for the determination of the amount of fresh charge added during the cycle. This iterative calculation differs insignificantly from the calculation of the pressure discontinuity at $\theta_o^{(+)} = 0$, which was described for the first specialization of the general model and detailed in equations (III-51) to (III-56). The fundamental cause of the difference is that the mass addition here is accompanied by a volume change, in contrast to the former situation where the volume was fixed. The volume change is expressible in terms of the compression ratio r and modifies only the expression for $\Delta \ln \rho$ in equation (III-52).

$$\Delta \ln \rho = \frac{\rho\left(\theta_o^{(+)}\right)(1+E_m)/r - \rho}{\rho} \tag{III-90}$$

This change in $\Delta \ln \rho$ produces changes in the definitions of $\tilde{b}$ and $\tilde{c}$ given in equation (III-53) by adding the compression ratio as a factor.

$$\tilde{b} = \frac{-r\rho}{\rho\left[\theta_o^{(+)}\right]} \left\{ 1 - \left(\frac{\partial \ln T}{\partial h} \right)_{p,n_\lambda} \left[h^{(0)} - {}^*H^\lambda n_\lambda^{(0)} \right] - \frac{\sum\limits_\lambda n_\lambda^{(0)} - \sum\limits_\lambda n_\lambda}{\sum\limits_T n_T} \right\}$$

$$\tilde{c} = \frac{r\rho}{\rho\left[\theta_o^{(+)}\right]} \left\{ \left(\frac{\partial \ln T}{\partial h} \right)_{p,n_\lambda} \left(h\left[\theta_o^{(+)}\right] - h^{(0)} \quad - {}^*H^\lambda \left\{ n_\lambda\left[\theta_o^{(+)}\right] - n_\lambda^{(0)} \right\} \right) + \frac{\sum\limits_\lambda n_\lambda\left[\theta_o^{(+)}\right] - \sum\limits_\lambda n_\lambda^{(0)}}{\sum\limits_T n_T} \right\} \tag{III-91}$$

No numerical quadrature need be carried out at this level of modeling, not even for work. Since the heat transfer is zero, equation (III-66) can be used to calculate the work from the changes in internal energy

$$\int p \frac{dV}{d\theta} d\theta = -\int d(Mu) = -\Delta(Mu) \tag{III-92}$$

for those portions of the cycle where there is no mass addition. This formula gives

$$\int_\pi^{3\pi} p \frac{dV}{d\theta} d\theta = -M(\pi)[u(3\pi) - u(\pi)] = -M(3\pi)\left\{ \left[u_1(3\pi) - u_1(\theta_0) \right] + \left[u_2(\theta_0) - u_2(\pi) \right] \right\} \tag{III-93}$$

as a special case by using $u(3\pi) = u_1(3\pi)$, $u(\pi) = u_2(\pi)$, and $u_1(\theta_0) = u_2(\theta_0)$. For those portions of the cycle where mass addition occurs, the pressure is constant and again numerical quadrature is unnecessary.

$$\int p \frac{dV}{d\theta} d\theta = p\, \Delta V \qquad \dot{p} = 0 \tag{III-94}$$

Performance Parameters

During a cycle calculation a number of functions are calculated which serve as indicators of cycle behavior. Foremost among these are the cycle work and heat transfer functions. The indicated work W_I, the pump work W_p, and the heat loss Q are cycle functions defined by integrals over the cycle

$$W_I(\theta)=\begin{cases} 0 & 0\le\theta\le\pi \\ \displaystyle\int_{\pi}^{\theta} p\frac{dV}{d\theta}\,d\theta & \pi\le\theta\le 3\pi \\ W_I(3\pi) & 3\pi\le\theta\le 4\pi \end{cases}$$

$$W_p(\theta)=\begin{cases} \displaystyle\int_{0}^{\theta} p\frac{dV}{d\theta}\,d\theta & 0\le\theta\le\pi \\ W_p(\pi) & \pi\le\theta\le 3\pi \\ W_p(\pi)+\displaystyle\int_{3\pi}^{\theta} p\frac{dV}{d\theta}\,d\theta & 3\pi\le\theta\le 4\pi \end{cases} \tag{III-95}$$

$$Q(\theta)=\int_0^{\theta}\left(\frac{\dot{Q}}{\omega}\right)d\theta$$

As defined here the functions $W_I(\theta)$ and $W_p(\theta)$ represent work done by the working fluid when they are positive and work done on the working fluid when they are negative. For a typical cycle $W_I(3\pi)>0$ and $W_p(4\pi)<0$. The function $Q(\theta)$ is the heat loss, and consequently $Q(4\pi)>0$ for a typical cycle. The average derivatives of these functions, over an interval $\Delta\theta$, are calculable by difference.

$$\begin{aligned} \frac{\Delta W_I}{\Delta\theta} &= \frac{[W_I(\theta+\Delta\theta)-W_I(\theta)]}{\Delta\theta} \\ \frac{\Delta W_p}{\Delta\theta} &= \frac{[W_p(\theta+\Delta\theta)-W_p(\theta)]}{\Delta\theta} \\ \frac{\Delta Q}{\Delta\theta} &= \frac{[Q(\theta+\Delta\theta)-Q(\theta)]}{\Delta\theta} \end{aligned} \tag{III-96}$$

During the combustion phase of the cycle the indicated work can be separated into contributions from the burned and unburned gases.

$$\begin{aligned} &W_1(\theta)=\int_{\theta_0}^{\theta} p\frac{dV_1}{d\theta}\,d\theta, \qquad W_2(\theta)=\int_{\theta_0}^{\theta} p\frac{dV_2}{d\theta}\,d\theta \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \theta_0\le\theta\le\theta^* \\ &W_1(\theta)+W_2(\theta)=W_I(\theta)-W_I(\theta_0), \qquad \frac{\Delta W_1}{\Delta\theta}+\frac{\Delta W_2}{\Delta\theta}=\frac{\Delta W_I}{\Delta\theta} \end{aligned} \tag{III-97}$$

In addition to the cycle functions just defined, one would like to have some measure of overall cycle behavior. One class of such indicators could be the increase in mass $\Delta M^{(+)}$ and species moles $\Delta n_{\lambda}^{(+)}$ brought about by the flow of fresh charge through the intake system because they represent the input per cycle to the engine.

$$\Delta M^{(+)} = M^{(+)}_{\max}$$

$$\Delta n^{(+)}_{\lambda} = M^{(+)}_{\max} n^{(0)}_{\lambda} \qquad \text{(III-98)}$$

$$M^{(+)}_{\max} \equiv \max[0, M^{(+)}(\theta)]$$

The expressions for $\Delta M^{(+)}$ and $\Delta n^{(+)}_{\lambda}$ take into account the definition of $M^{(+)}(\theta)$. That definition (see the discussion following equation (I–117b)) introduced a discontinuity into $M^{(+)}$ at its maximum value as shown in the sketches for figure 2, which illustrate the range of intake and exhaust flow behavior which can be accommodated. The formulas also presuppose that $M^{(+)}$ changes from negative to positive values only once. The product of $\Delta n^{(+)}_{\lambda}$ with the molecular weight of species λ, $\mathcal{W}_{\lambda}$, gives the mass input $\Delta m^{(+)}_{\lambda}$ of this species. Summation of this over a subset of species gives the mass addition ascribable to those species. Mean mass flow rates of fresh charge and species to the cylinder can be calculated from mass increments simply by dividing them by the time for one cycle $4\pi/\omega$.

$$<\dot{M}^{(+)}> \equiv \frac{\omega \, \Delta M^{(+)}}{4\pi}$$

(III-99)

$$<\dot{M}^{(+)}_{\lambda}> \equiv \frac{\omega[\Delta n^{(+)}_{\lambda}]\mathcal{W}_{\lambda}}{4\pi} \qquad (\lambda \text{ not summed})$$

The exhausted mass and the moles of each species exhausted for each cycle are calculated similarly.

$$\Delta M^{(-)} = M^{(-)}_{\max} - M^{(-)}[\theta^{(-)}_{c}]$$

(III-100)

$$\Delta n^{(-)}_{\lambda} = \Delta M^{(-)} n^{(e)}_{\lambda}$$

$$M^{(-)}_{\max} \equiv \max[0, M^{(-)}(\theta)]$$

The mean mass flow rates of exhaust and species from the cylinder can be calculated analogously to equation (III-99).

$$<\dot{M}^{(-)}> = \frac{\omega \, \Delta M^{(-)}}{4\pi}$$

(III-101)

$$<\dot{m}^{(-)}_{\lambda}> = \frac{\omega\left(\Delta n^{(-)}_{\lambda}\right)\mathcal{W}_{\lambda}}{4\pi} \qquad (\lambda \text{ not summed})$$

Finally, the mean net mass flow rates for the intake and exhaust systems are defined as

$$<\dot{M}^{(\pm)}>_{\text{net}} \equiv \frac{\omega}{4\pi}\int_{\theta^{(\pm)}_{o}}^{\theta^{(\pm)}_{c}} \dot{M}^{(\pm)}(\theta)\,d\theta \qquad \text{(III-102)}$$

An important measure of the mechanical efficiency of an internal combustion engine is the efficiency with which it converts chemical energy to useful mechanical energy. But to calculate such an efficiency, one must have some measure of the energy content of the working fluid. A reasonable choice for this value is the enthalpy difference between the enthalpy of the working fluid for the composition at intake valve closing $\theta_c^{(+)}$ and the enthalpy of the same working fluid but for an equilibrium composition. Both enthalpies are calculated for the same temperature and pressure. If the temperature and pressure are chosen as the nominally ambient values of $T = 298.15$ K and $p = p_e$, then the chemical energy per unit mass may be defined as

$$\Delta h_{CE} \equiv h(T,p,n_\lambda) - h^{(eq)}(T,p) \qquad T = 298.15\,K,\ p = p_e,\ n_\lambda = n_\lambda\left(\theta_c^{(+)}\right) \tag{III-103}$$

where the last term is the enthalpy at equilibrium conditions. The chemical energy is a measure of the available energy per unit mass of working fluid and can be used in the definition of three parameters to characterize the distribution of available energy among useful mechanical work, heat loss to the coolant, and energy content of the exhaust gas. These three parameters will be termed efficiencies. The net work efficiency η_{net} is the ratio of the net work to the available energy. The heat loss efficiency η_Q describes the capability of the coolant to extract energy from the working fluid. It is the ratio of the cycle heat loss to the available energy.

$$\eta_{\text{net}} \equiv \frac{\left[W_I(4\pi) + W_p(4\pi)\right]}{M\left[\theta_c^{(+)}\right]\Delta h_{CE}}, \qquad \eta_Q = \frac{Q(4\pi)}{M\left[\theta_c^{(+)}\right]\Delta h_{CE}} \tag{III-104}$$

The ability of the working fluid to retain its energy content will be described by the exhaust efficiency η_{exh}. It will be defined as the ratio of the energy content of the composite exhaust gas to the available energy.

$$\eta_{\text{exh}} \equiv -\frac{(\Delta h_{\text{exh}})M^{(-)}\left[\theta_c^{(-)}\right]}{M\left[\theta_c^{(+)}\right]\Delta h_{CE}} \tag{III-105}$$

The quantity Δh_{exh} is the difference between the enthalpy of the composite exhaust gas and its enthalpy at equilibrium for $T = 298.15\,K$ and $p = p_e$. The heat loss and exhaust efficiencies represent energy losses, and hence inefficiencies, from the point of view of the engine. Obviously the three efficiencies defined here need not total unity, but often their sum is quite close to that value.

The indicated work, pump work, heat loss, and exhaust energy can also be expressed as average power over a cycle. If P_I, P_p, P_Q, and P_{exh} are the indicated power, the pump power, the heat loss power, and the exhaust power, then

$$P_I \equiv \frac{\omega W_I(4\pi)}{4\pi}, \qquad P_p \equiv \frac{\omega W_p(4\pi)}{4\pi}$$

$$P_Q \equiv \frac{\omega Q(4\pi)}{4\pi}, \qquad P_{\text{exh}} \equiv \frac{-\omega M^{(-)}\left[\theta_c^{(-)}\right]\Delta h_{\text{exh}}}{4\pi} \tag{III-106}$$

are their defining equations. Oftentimes the indicated work and pump work are given in units of pressure and called mean effective pressures. These are obtained by dividing the work by the displacement volume V_d, which is defined as

$$V_d \equiv V(\pi) - V(0) \tag{III-107}$$

and hence

$$\mathrm{IMEP} \equiv \frac{W(4\pi)}{V_d}, \quad \mathrm{PMEP} \equiv \frac{W_p(4\pi)}{V_d} \tag{III-108}$$

where IMEP is the indicated mean effective pressure and PMEP is the pump mean effective pressure. Finally the net work for the cycle may be expressed as a mean torque $\mathfrak{J}$. It is calculated as the net work for the cycle divided by the radians per cycle.

$$\mathfrak{J} \equiv \frac{W_I(4\pi) + W_p(4\pi)}{4\pi} \tag{III-109}$$

Fresh Charge Specification

The fresh charge fed to the cylinder is formed from three streams: air, fuel, and recirculated exhaust gas. The recirculated exhaust gas which is used in a given cycle is assumed to be the composite exhaust gas from the preceding cycle. Its contribution to the fresh charge, expressed as a mass fraction of the fresh charge, is designated by E_G. Its state, prior to its incorporation in the fresh charge, is defined by the exhaust pressure p_e and a temperature which might be the mean exhaust temperature but could also be some other arbitrarily assigned temperature. The initial state of the air and fuel is defined by a fuel pressure p_f, the air temperature, and the (partial molar) enthalpies of the fuel constituents. The fuel constituents are not restricted to chemical species which have traditionally been regarded as fuels, namely, hydrocarbons. The label "fuel" is only used to distinguish reactants from the principal oxidizer, which is assumed to be air. The relative proportion of air to fuel is given by the air-fuel mass ratio A/F. The air itself is a mixture of "dry" air with an empirical formula

$N_{1.56168}O_{0.41959}Ar_{0.009365}C_{0.000319}$

and water vapor. The empirical formula for dry air corresponds to the mole fractions 0.78084, 0.209476, 0.009365, and 0.000319 for N_2, O_2, Ar, and CO_2, respectively. The water content is specified by the relative humidity, the ratio of the humidity to the humidity at saturation. The humidity is the mass of water vapor per mass of dry air.

The fresh charge is formed from the fuel, air, and exhaust gas in two stages. In the first stage the fuel is mixed with the air at a fixed enthalpy and pressure with the assumption that all liquid fuels vaporize in the mixing process. The pressure of the air-fuel mixture is then changed from p_F to the manifold pressure p_m by one of the two processes (I-118). In the second stage the pressure of the composite exhaust gas is changed from p_e to p_m by one of the two processes (I-118), and the resulting gas is mixed with the fuel-air mixture at fixed enthalpy and manifold pressure to produce the fresh charge mixture to be used in the cycle calculations.

For those cycle calculations which correspond to the three specializations of the general model, it is possible to characterize the makeup of the working fluid by giving the mass fractions contributed by fuel x_F, air x_A, recirculated exhaust gas x_E, and residual exhaust gas x_R. These mass fractions are expressible in terms of A/F, E_G, and $E_m(\pi)$.

$$x_F = \frac{(1 - E_G)E_m(\pi)}{(1 + A/F)\left[1 + E_m(\pi)\right]}, \quad x_A = (A/F)x_F$$

$$x_E = \frac{E_G E_m(\pi)}{1 + E_m(\pi)}, \quad x_R = \frac{1}{1 + E_m(\pi)} \tag{III-110}$$

For these same cycles it is also possible to calculate two simple measures of efficiency of the cylinder charging process. One of these is the volumetric efficiency η_V, which is the fraction of the total volume available to the fresh charge. The other is the mass efficiency η_M, which is the fraction of the total working fluid mass contributed by the fresh charge.

$$\eta_V \equiv \frac{V(\pi) - V[\theta_o^{(+)}]}{V(\pi)} = 1 - \frac{V[\theta_o^{(+)}]}{V(0)} \frac{V(0)}{V(\pi)} = 1 - \frac{\rho(0)}{\rho[\theta_o^{(+)}]} r^{-1}$$

$$\eta_M = \frac{M(\pi) - M[\theta_o^{(+)}]}{M(\pi)} = \frac{E_m(\pi)}{1 + E_m(\pi)} \tag{III-111}$$

Properties Representations

The temperature dependence of the thermodynamic and transport properties must be known to carry out cycle calculations. The temperature dependence is assumed to be expressible as a polynomial in the temperature or its reciprocal and, for some properties, an additional logarithmic term. The thermodynamic properties for each species take the form

$$\frac{d({}^*H/R)}{dT} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{{}^*H}{RT} = a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T} \tag{III-112}$$

$$\frac{{}^*S}{R} = a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7$$

where the species label has been suppressed. The viscosity of each species takes the form

$$\ln \eta = a_1 \ln T + \frac{a_2}{T} + \frac{a_3}{T^2} + a_4 \tag{III-113}$$

where again the species label has been suppressed. The expression for the thermal conductivity is identical in form to that for the viscosity.

Chapter IV

Organization and Use of Computer Program ZMOTTO

Bonnie McBride and Frank J. Zeleznik

The analysis of Chapters I to III has been translated into a large, complex, general-purpose Fortran IV computer program called ZMOTTO. This chapter gives a general description of the program capabilities, a detailed description of the input, several examples, and a brief description of each subroutine.

The program contains not only the general model but also the three specializations of that model. The computer program has been written to permit multicycle calculations at five levels of complexity ranging from a purely thermodynamic model to a very general model which can cope with valve timing and combustion kinetics. While the program uses thermodynamic, transport, and chemical kinetic properties, it has been constructed to make data corrections, additions, and deletions simple and convenient.

Because of the very many options available, a user is faced with an almost bewildering array of choices. To assist the user, we shall present several examples of calculations designed to illustrate input data structure, computational capabilities, and computational times. Because it is virtually impossible to demonstrate all of the many options, we have selected examples which show the effects of either important phenomena or simplifying assumptions. We will also provide brief descriptions of the various routines, their functions, and their interrelationships.

Because of the mammoth size of the computer program (approximately 10 000 card images) we have found it impractical to describe much of its fine structure. In many cases it is this fine structure which permits the calculations to be performed reliably, accurately, expeditiously, and economically. We seriously caution everyone to avoid even apparently trivial program changes. Many of the numerical procedures have been developed to deal safely with even the most difficult problems. A change which might appear to have been safely and correctly made for a particular problem could surface at a later time and easily cause serious errors in some seemingly unrelated calculation. We ourselves approach program changes with some trepidation because of the highly coupled and "multiple use" nature of many of the routines. We cannot promise that the program is totally free from error or that it can successfully solve all possible problems that it might be asked to do. We have, however, tested it successfully on many kinds of extremely difficult problems. But our personal experience has shown that even after many years of extensive use a complex program may contain undiscovered errors or may encounter unanticipated situations with which it cannot cope. We have tried to keep such problems to a minimum by always erring on the side of safety and accuracy rather than computational speed. Even so the computer program is capable of performing calculations with surprising speed.

When it becomes necessary to refer to particular program variables in the discussion to follow, this will be done with the symbols used in the computer program rather than the mathematical symbols of Chapters I to III. A translation between mathematical symbols and computer symbols is supplied as part of tables IV to VI for the input variables. Some other computer variables will be identified in the discussions of the various routines.

Program Capabilities

The ZMOTTO program calculates Otto cycle performance parameters as well as working fluid compositions and properties throughout the cycle for a number of consecutive cycles and for a variety of input parameters. This section gives an overview of the program capabilities; details are given in subsequent sections. The calculations take place at five levels of sophistication. The higher the level, the more complex the model, the more input required, and the more computer time used. A calculation cycle is defined to be an interval of 720 crankangle degrees beginning at top dead center (TDC). Program execution produces results for a sequence of calculation cycles, hereinafter referred to as a case.

The first few cycles calculated in a particular case are always the third specialization of the general model. They are the lowest level of sophistication and will be referred to as level 1 cycles. These cycles will sometimes also be called ideal cycles. All higher level cycles must be preceded by the ideal cycles, which can be thought of as providing initial estimates of residual exhaust gas properties. All higher levels of sophistication include heat transfer and will be termed nonideal cycles.

A case may contain several levels, but the levels of complexity cannot decrease with cycle number. Fuel and engine characteristics remain constant for a given case, but many parameters are allowed to vary from cycle to cycle for nonideal cycles. A typical case will always include a number of ideal cycles and may also contain nonideal cycles. The number of ideal cycles varies depending on how long it takes for the exhaust temperature and composition to reach a steady state. The nonideal cycles following these ideal cycles are counted separately. The first nonideal cycle is called cycle 1. The number of nonideal cycles is variable and is specified in the input data.

Data are dumped at the end of each nonideal cycle and may later be used for restarting the case or for plotting many of the output variables throughout each cycle. The ZMOTTO program is capable of restarting a case, but a separate program is required for plotting. Users must supply their own plotting routines because graphics capabilities vary considerably from installation to installation.

A particular sequence of cycles (case) is shown schematically in figure 1. A brief description of the modeling levels is given in the following paragraphs and is summarized in figure 2. A more detailed description is available in Chapters I and III.

The input information required by the program is determined by the modeling level and is of two types. The first type is the physical properties data for the working fluid. It includes thermodynamic,

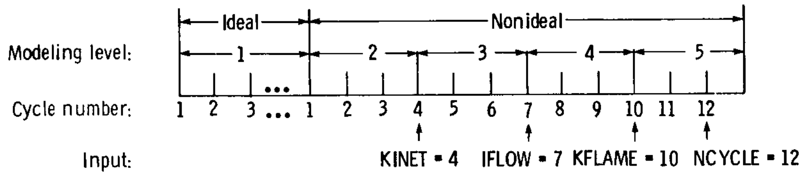


Figure 1. - Cycle numbering example.

Feature	Modeling level				
	5	4	3	2	1
Flow	Poppet valve formulas		Zero-pressure-drop flow; flow reversal only at $\theta = 0$ or $\theta = 3\pi$, where discontinuities are possible		
Flame	Kinetic	Equilibrium			
Flame propagation	Mass burning formulas				Instantaneous
Burned-gas chemistry	Finite rate			Equilibrium	
Heat transfer	Nonzero				Zero

Figure 2. - Modeling levels.

transport, and chemical kinetic properties for the constituents of the working fluid. The second type is all other input data necessary to define a given case and will be referred to as case input data. Case input data will define the geometric and operating characteristics of the engine as well as the modeling levels for a case.

Level 1, Third Specialization Model (Ideal Cycle)

Level 1 cycles are not optional and are computed at the beginning of each case. They have equilibrium chemistry, constant volume combustion, and no heat transfer. Calculations do allow for residual gas effects, exhaust gas recirculation (EGR), spark advance, supercharging, and throttling. Operating conditions are not permitted to change during these cycles.

For a case without supercharging it is assumed that the intake valve opens at the point where the pressure equals the manifold pressure PMFOLD. When PMFOLD>PEXH (exhaust pressure), a supercharging case, the intake valve opens at 0°. The intake valve always closes at 180°. The exhaust valve opens at 540° and closes at 720°. A steady state is assumed to have been reached when the exhaust gas temperature agrees with the previous cycle value within 1 degree Kelvin. Also the exhaust compositions expressed in mole fractions must agree within 0.01 percent on successive ideal cycles.

This model requires only thermodynamic data in addition to the case input data. A typical calculation time on the IBM 370/3033 is 1/4 second or less per cycle. It takes anywhere from 3 to 12 cycles to reach a steady state.

Level 2, Second Specialization Model (Equilibrium Chemistry and Heat Transfer)

Level 2 cycles have heat transfer, finite-rate burning, and equilibrium chemistry in addition to the capabilities of the level 1 cycles. This level is optional, but if used, it would be the first nonideal cycle starting with residual gas from the ideal cycles.

The only physical properties data needed in addition to the thermodynamic data required for level 1 are transport properties data for some of the non-Eichelberg heat transfer coefficient options. For these options the HC2 constant is not equal to zero in equation (I-105).

A calculation time on the IBM 370/3033 is typically 2 to 4 seconds per cycle for the level 2 model.

Level 3, First Specialization Model (Chemical Kinetics and Heat Transfer)

Level 3 cycles have all of the capabilities of level 2 except that chemical kinetics replaces equilibrium chemistry in the burned gas during burning and expansion. The chemical kinetic data are an additional input requirement.

A typical calculation time on the IBM 370/3033 might be 5 to 7 seconds per cycle for a moderately complex burned-gas reaction mechanism such as given in the examples in the appendixes.

Level 4, General Model with Equilibrium Flame

Level 4 cycles have valve timing, with flow through the valves calculated by using the poppet valve equations (I-110) and (I-117). Chemical kinetics in the burned gas is assumed to govern the chemistry from the start of combustion until the intake valve opens. The properties of the flame front are assumed to be equilibrium properties.

The poppet valve flow equations require shear viscosity data for calculating the Reynolds number (eq. (I-116)). Thus for levels 4 and 5 the viscosity data must be included even for the Eichelberg heat transfer coefficient, which does not use transport properties data. Also for these models many more case input data are required for the poppet valve flow parameters in equations (I-110) and (I-117).

A typical calculation time on the IBM 370/3033 is of the order of 10 to 15 seconds per cycle.

Level 5, General Model with Kinetic Flame

Level 5 cycles have only one additional complication from level 4: a kinetic flame is assumed during combustion. That is, unburned gas is injected directly into the burned gas during combustion without first attaining a chemical equilibrium state. Additional chemical kinetic data are required for the breakdown of the fuels.

A typical calculation time is about 1 minute for a level 5 cycle on the IBM 370/3033.

Input and Output Data Files

Input and output data files and logical input/output units are listed in table I. Generally in a particular computer run, only input data required for the modeling level need to be included. The thermodynamic properties file (unit 4) is always required input. The transport properties (unit 8) and chemical kinetic data (unit 9) files will sometimes be required. The case input data (unit 5) are the data that vary from case to case. The case output data file (unit 6) is the main printed output for all cases. The file on unit 7 is a dump of the common variables for restart or plotting.

The input and output data files will be discussed in the following sections. Sample input and output are given with the examples as discussed in the section Typical Examples of Problems. Although the input files may be either card decks, tape files, disk files, or some combination, a data file record will often be referred to as a card.

Input

Thermodynamic data. – Thermodynamic data are required for all modeling levels. The pure species properties have the same empirical form as the properties used with the Gordon-McBride CEC program (ref. 1), see equation (III–112). The mixture properties are described by equations (I–130) to (I–137). The format and a sample set of data including references are given in appendix A to this chapter. The CEC program only requires data for the reaction products, but ZMOTTO also requires data for the fuels. The card format for ZMOTTO is identical to that used with CEC with one exception. An optional word was added to the first card of a species set in columns 17 and 18. This word may be used to distinguish among species with the same empirical formula such as the isomeric species normal butane and isobutane.

The program expects to read the data from logical unit 4. Only data for the chemical system related to the case are stored, even though logical unit 4 may contain other data. Although program dimensions allow for 80 species, some storage is preempted for air and other special mixtures. Also the dimensions for the numerical integration routines allow for 75 differential equations with 72 available for species. As a result no more than 76 species should be included in calculations for levels 1 and 2 and 72 species for levels 3 to 5 including fuels. Different phases of the same species are counted separately. The order of the data is

(1) A card giving the temperature intervals
(2) Data for all species which are products of reaction
(3) A card with END in columns 1 to 3
(4) Data for the fuels
(5) A card with END2 in columns 1 to 4

The data must include the following species:

(1) Thermodynamic data for the constituents of air, namely N_2, O_2, Ar, and CO_2, must be included among the reaction product species. The air composition is given in the section Fresh Charge Specification of Chapter III.

(2) If relative humidity is given in the input, data for liquid and gaseous water should be included with the products.

(3) If some products are also fuels, the thermodynamic data for these species must be included with both the products and the fuels.

(4) For levels 3 to 5, data for all of the species in the chemical reaction mechanism must be included in the thermodynamic data for the reaction products and with the same name.

(5) If there are multiple condensed phases of a product species, they must appear consecutively in either ascending or descending order according to temperature.

(6) If there are liquid fuels in the case input, it is not necessary to have thermodynamic data for the liquids if (partial molar) enthalpies are included with the case input. However, gaseous data must always be available. If there are data for the liquid fuels, then the gaseous data for a particular species must immediately follow the liquid data for the species in the fuel group. A discussion of enthalpy and enthalpy base is given in reference 1.

Transport properties. – Transport data are only required for certain options in the case input. Shear viscosities and thermal conductivities of gaseous species, reaction products and fuels, are used for some of the non-Eichelberg heat transfer coefficient options available for levels 2 to 5 (eq. (I-105) with HC2 not equal to zero). Shear viscosities are also used for levels 4 and 5 in calculating Reynolds number (eq. (I-116)) for poppet valve flows.

The pure-species gaseous properties are in the empirical form given in equation (III-113). The format, data references, and listing of some data are given in appendix B to this chapter. Mixture properties are calculated by equations (I-152) to (I-155).

The program expects the data to be on logical unit 8. When the appropriate options appear in the case input, it will read and store any data with a name matching a name in the thermodynamic data. Program dimensions allow for as many as 30 species. If thermal conductivities or viscosities data are missing for a species, the program uses zero for the property. If data for more than 30 species are available, only data for the first 30 species in the system will be used.

Chemical kinetic data. – Chemical kinetic data for gaseous species are required for levels 3 to 5. Equations for reactions, stoichiometric coefficients, third-body efficiencies, and rate constants are given in equations (I-138) to (I-145). The card format for the data is similar to that used with the kinetics program GCKP of Bittker and Scullin (ref. 2), but there are some differences. The format, order, data references, and sample data listings are given in appendix C to this chapter.

The program expects the data to be available on logical unit 9 for the level 3, 4, and 5 calculations. Program dimensions allow for 200 reactions in the mechanism and up to 72 species. Exceeding these values causes termination of the calculation. Species names must match names in the thermodynamic data.

All species appearing in the thermodynamic data but not in the chemical kinetic reaction mechanism are assumed to be nonreacting. At levels 3 and 4 the reaction mechanism need only involve the burned-gas species. At level 5 the mechanism must involve all species, including the reactants. No provision has been made for the occurrence of condensed species, such as graphite, during chemical kinetic calculations. Their appearance will lead to a termination of the computations.

Case input. – Case input data are used to specify working fluid composition, engine geometry, operating characteristics, intake and exhaust characteristics, and modeling level. The case input including data order is summarized in table II. The data file, which is read from logical unit 5, may contain data for any number of case input sets. Program variables are initialized between cases.

Reactant cards: These cards follow a card with REAC in columns 1 to 4 at the beginning of the data file. The format of the cards is given in table III. It is similar to the one used in the CEC program (ref. 1). However, a new variable was added to columns 79 and 80 to distinguish among species with the same empirical formula. This two-letter word must match columns 17 and 18 on the first card of the thermodynamic data for the fuel. All reactants which are read in will be treated as fuels with respect to the fuel-air mixtures specified in the AFINP namelist even though some reactants might be oxidizers. Air is automatically added to the reactants by the program.

OMIT cards: OMIT cards are the cards with OMIT in columns 1 to 4. They are optional and provide a means for eliminating species from consideration as reaction products without physically altering the thermodynamic data file. The portion of the name in columns 17 and 18 of the first thermodynamic data card for each species is not included with the names on these cards. Thus one name on an OMIT card will omit all species whose names differ only by the contents of columns 17 and 18.

OTTINP namelist: OTTINP is the first namelist read. It follows a card with NAME in columns 1 to 4. The variables and definitions are listed in table IV. Parameters which are set in the OTTINP namelist remain unchanged throughout the calculations for a case. Thus this namelist appears only once in the initial data file.

AFINP namelist: This namelist contains the variables which are allowed to change between nonideal cycles. There may be several AFINP namelists for a particular case. They are read between the cycles and generally change the calculations for the next cycle. The variables are listed and defined in table V. One logical variable VARAF indicates whether another namelist should be read before calculating the next cycle. If VARAF is false, no more AFINP namelists are read and the parameters remain unchanged. Then if NCYCLE is greater than the current nonideal cycle number, calculations will continue until the cycle number NCYCLE. If VARAF is true, then another AFINP namelist will be read on the next cycle. Levels 3, 4, and 5 are indicated by setting certain case input variables to the cycle where the level is to begin. The variables KINET, IFLOW, and KFLAME are starting cycle numbers for levels 3, 4, and 5, respectively (table V). If none of these variables are set or if they are set to cycle numbers greater than 1, then level 2 is assumed if NCYCLE is greater than or equal to 1. Figure 1 illustrates a case calling for three cycles at each nonideal level. Complications can arise in the transition from level 2 or 3 to level 4 or 5 when the air-fuel ratio is changing as indicated in the next paragraph.

FLOWIN namelist: This namelist contains parameters which are used for levels 4 and 5 only. It must follow the first AFINP namelist which contains a value for IFLOW or KFLAME. The FLOWIN namelist contains crankangles giving the valve timing and variables in the poppet valve equations (I-110) to (I-117). The variables are listed and defined in table VI. For levels 4 and 5 the crankangles at which the intake and exhaust valves open and close are given in the FLOWIN namelist as IVOPEN, IVSHUT, EVOPEN, and EVSHUT. The valve timing will usually be different from that prescribed for the lower levels of sophistication. This can lead to a transition problem between the lower levels and the higher levels. The problem occurs when the intake valve opens before the end of the calculation cycle (before 720°) because the air-fuel mixture is being changed with AFINP namelist at 0°.

To solve this problem, for the first level 4 (or 5) cycle, we let the intake valve open at 0° since the calculation is already beyond the requested valve opening location. We also reopen the valve, as requested, near the end of this cycle. The same air-fuel mixture will be used throughout the calculation cycle, even after the intake valve opens near the end, since a new one cannot be read until the calculation again reaches 0°. If a new mixture is then read from an AFINP namelist, at the beginning of the second level 4 (or 5) cycle, it will be ignored until the intake valve opens near the end of this second cycle. Then the second mixture value will be used in making up the incoming charge for the remainder of the second cycle and as long as the intake valve remains open at the beginning of the third cycle. Figure 3 illustrates a sample case where the intake valve opening $\theta_o^{(+)}$ occurs before 720°.

Restart input: Data from I/O units 5 and 7 (table I) are used as input for a restart run. Unit 5 contains case input, and unit 7 contains data dumped at the end of each nonideal cycle in one or more previous runs.

The case input for restart is abbreviated as indicated in table II. The first card contains RESTART in columns 1 to 7 and will be referred to as a RESTART card. The RESTART card may contain an integer indicating the cycle number where the calculations are to be restarted. This may be a cycle which was calculated in the previous run. If no integer is given, calculations will continue from the last cycle completed. The RESTART card is followed by at least one AFINP namelist. To restart the calculations, the first namelist must include VARAF = T or NCYCLE set to some number greater than or equal to the restarting cycle. A FLOWIN namelist will be required to follow any AFINP namelist for which $IFLOW \neq 0$ and for which all previous cycles were at levels less than 4.

The data on I/O unit 7 are data from labeled COMMON which were dumped one nonideal cycle at a time in the previous run or runs. These data are read in, one cycle at a time, until the point is reached where the calculations are to resume. Calculations simply continue from that point. The dumps on unit 7 continue at the end of each newly calculated cycle, possibly overwriting previous data.

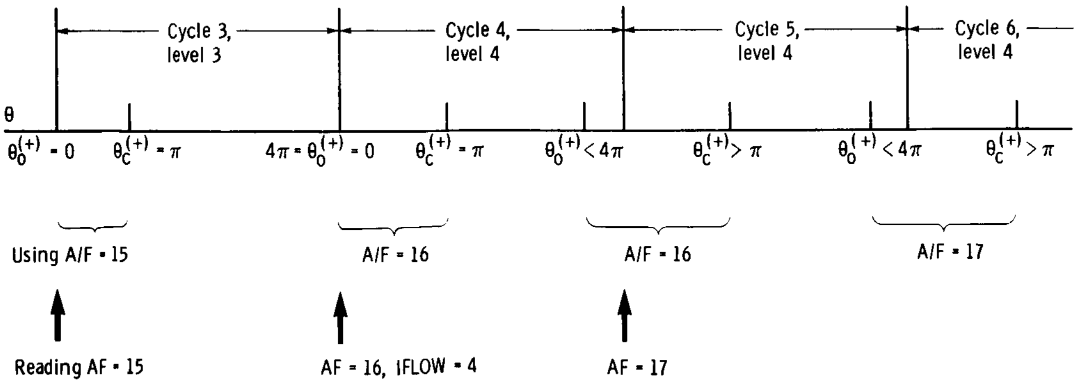


Figure 3. - Cycle-to-cycle variation in air-fuel ratio.

The sequence of cycles shown in figure 1 could have been run in two or more passes. For example, to split it into two passes of six nonideal cycles each, the initial run would have NCYCLE = 6 and the restart run would have NCYCLE = 12. Since poppet-valve flow starts after the restart for this case, IFLOW and KFLAME could be set in either pass or in both passes. If it is then desired to redo cycles 11 and 12 with different burning intervals, one would set restart at 11 and reset THBURN (the burning interval) in the AFINP namelist. Cycles 11 and 12 would be recalculated. The data dumped on unit 7 would contain labeled common data from the previously calculated first 10 cycles followed by data for the newly calculated cycles 11 and 12.

Output

Output data files are indicated in table I. Output to be printed is written on logical unit 6. Unit 7 contains unformatted information for input and output. ZMOTTO writes information on unit 7 which may be read later by ZMOTTO to restart the program. This data file on unit 7 may also be used for plotting, see the section *Plot and restart dump.*

Most of the output is self-explanatory and will not be discussed in any great detail. See the section Examples of Typical Problems for illustrations of the output.

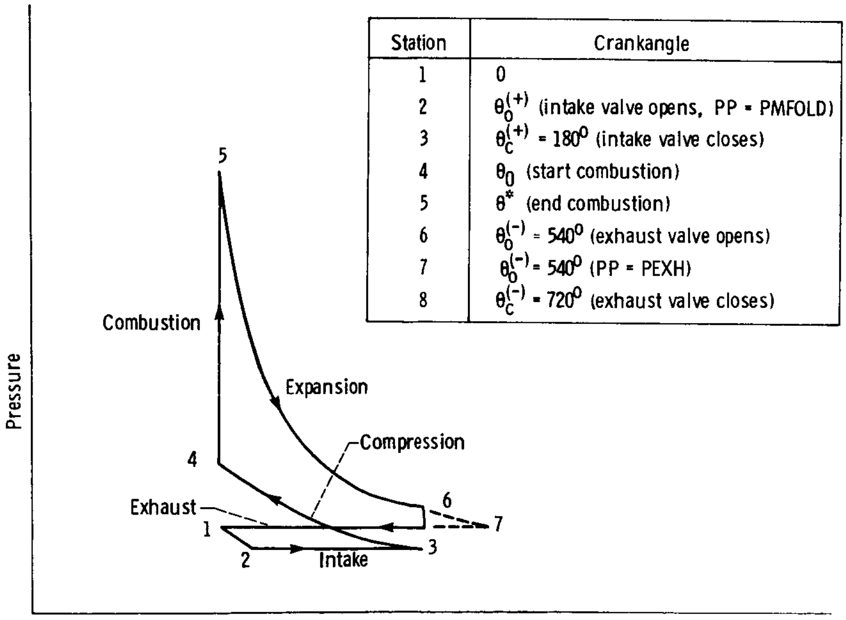
Case output. – The case output on logical unit 6 includes the following items:

(1) All input data are printed except the thermodynamic data. For the thermodynamic data only the species names along with a reference code and date are printed.

(2) Some intermediate data printed by the equilibrium routines are the same as the output for the CEC program (ref. 1).

(3) The output for level 1 cycles is given at special points in the ideal cycle identified as stations and labeled with station numbers. The station numbers are defined in an ideal indicator diagram shown in figure 4. Normally only the results for the last level 1 cycle are printed. Results for the other level 1 cycles can be requested with either the DEBUG or IPRINT variables in the AFINP namelist. Column one of the output gives the properties of the fresh charge at manifold conditions. For the last level 1 cycle, column 8 gives the equilibrium properties of the working fluid at station 4 but evaluated at the exhaust pressure and 298.15 K. These properties are used for calculating the chemical energy.

(4) For intermediate output on nonideal cycles, many variables at many crankangles throughout the cycle are printed. As with the level 1 cycles, special points throughout the cycles are called stations



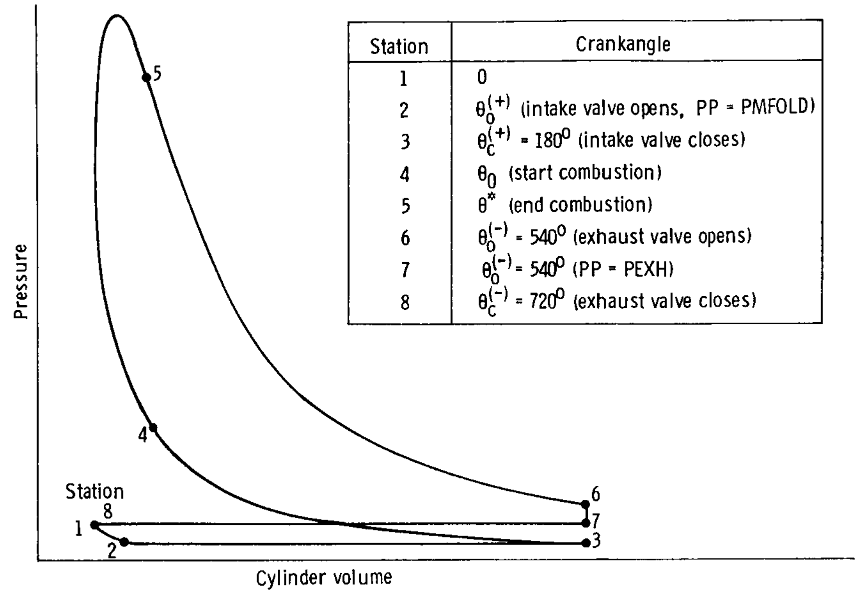
Station	Crankangle
1	0
2	$\theta_0^{(+)}$ (intake valve opens, PP = PMFOLD)
3	$\theta_c^{(+)} = 180^0$ (intake valve closes)
4	θ_0 (start combustion)
5	θ^* (end combustion)
6	$\theta_0^{(-)} = 540^0$ (exhaust valve opens)
7	$\theta_0^{(-)} = 540^0$ (PP = PEXH)
8	$\theta_c^{(-)} = 720^0$ (exhaust valve closes)

Figure 4. - Stations for modeling level 1.

and numbered. These stations for the various modeling levels are defined and marked on typical indicator diagrams in figures 5 and 6.

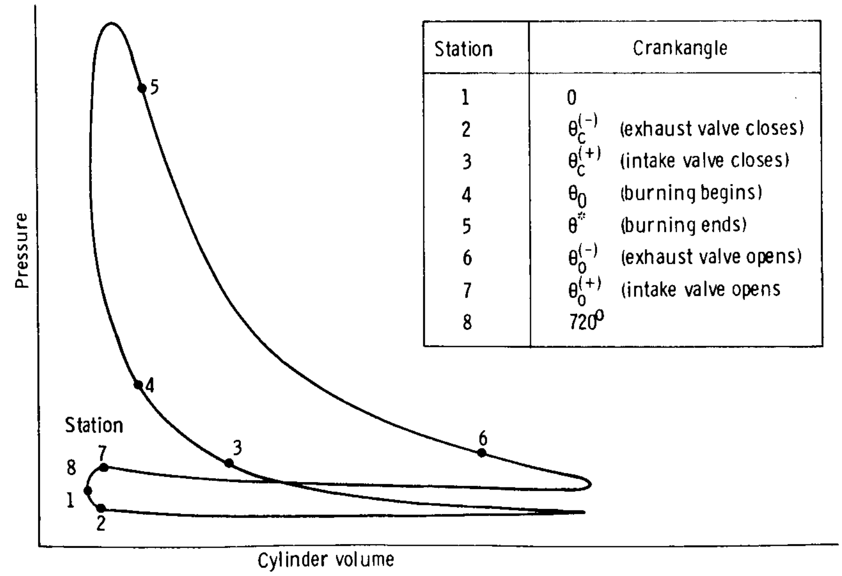
(5) A summary sheet of information at the end of each nonideal cycle includes some input information, performance parameters (as defined in the section Performance Parameters of Chapter III), and compositions of both the composite exhaust gas and the fresh charge.

(6) Error messages are largely self-explanatory and include the name of the program subroutine where they are printed. After some errors, calculations are discontinued, program flow returns to the main program, and the COMMON variable NPROC is 1 rather than −1 as it is for a normal completion. This information might be useful for printing a message at a computer terminal.



Station	Crankangle
1	0
2	$\theta_0^{(+)}$ (intake valve opens, PP = PMFOLD)
3	$\theta_c^{(+)} = 180^0$ (intake valve closes)
4	θ_0 (start combustion)
5	θ^* (end combustion)
6	$\theta_0^{(-)} = 540^0$ (exhaust valve opens)
7	$\theta_0^{(-)} = 540^0$ (PP = PEXH)
8	$\theta_c^{(-)} = 720^0$ (exhaust valve closes)

Figure 5. - Stations for modeling levels 2 and 3.



Station	Crankangle
1	0
2	$\theta_c^{(-)}$ (exhaust valve closes)
3	$\theta_c^{(+)}$ (intake valve closes)
4	θ_0 (burning begins)
5	θ^* (burning ends)
6	$\theta_0^{(-)}$ (exhaust valve opens)
7	$\theta_0^{(+)}$ (intake valve opens
8	720^0

Figure 6. - Stations for modeling levels 4 and 5.

Plot and restart dump. – The contents of most of the labeled COMMON are dumped on logical unit 7 at the end of each nonideal cycle. These data may be used for restarting a problem or for plotting. Each record contains all the COMMON data at 720 crankangle degrees. Cycle numbers coincide with the record numbers.

All variables in COMMON PLTS which can be used for plotting purposes are listed and defined in table VII. The few variables which appear in this COMMON and not in table VII are used for other purposes. The program subroutine DUMPCM should be used as a model for reading the COMMON data from logical unit 7. Also subroutine PLT should be used to get the order and dimensions of the variables in COMMON PLTS.

Examples of Typical Problems

We are now ready to discuss the results of some sample calculations carried out with the computer program ZMOTTO on an IBM 370/3033 computer. We cannot possibly explore and demonstrate all facets of the computer program. However, in showing and discussing some selected examples we have multifold purposes: (1) to display typical program input and output, (2) to illustrate some of the program capabilities and options, (3) to point out the effect of simplifying assumptions, and (4) to indicate the relative costs of various levels of modeling. It is not our intention, in these examples, to deal with any particular engine or mode of operation. We shall choose input parameters solely on the basis that they are loosely representative of the potential range of values one might encounter in typical problems. Our choice of parameters will sometimes produce highly aberrant cycle behavior.

We shall limit ourselves to six examples, each of which will differ in some measure from the others. The input data for these examples are of two types. In the first category are the thermodynamic, transport, and chemical kinetic properties of the constituents of the working fluid. These were described in previous sections and are illustrated in appendixes A to C. The second category of input information is used to specify working fluid composition, engine geometry, operating characteristics, intake and exhaust characteristics, and modeling level. These data were discussed under case input. The case input for the six cases we will use as sample problems is shown in appendixes D to I, together with some results of the calculations.

The results for the six sample problems will be illustrated by presenting selected segments of computer printout and computer-generated plots. These plots are drawn by connecting plotting points with straight line segments. The straight line segments are apparent on a few of the plots. These do not reflect the smoothness of the calculation but rather reflect both the number of points saved for plotting and the scale of the plots.

Example I (Cases 512 and 513; Levels 1, 2, and 3)

This example is a typical multicycle computation, at three modeling levels (KINET = 4, NCYCLE = 8), for the combustion of a lean mixture of fuel (PHI = 0.725) and humid air (RHUMID = 55). The fuel itself is a mixture of three liquid hydrocarbons: n-octane (C_8H_{18}), toluene (C_7H_8), and benzene (C_6H_6) at 0.984 atmosphere (PFUEL = PEXH = 0.984) and 298.15 K. The heat transfer coefficient is of the Eichelberg form (eq. (I-105)), with velocity (eq. (I-108)) chosen as the mean piston speed (HC1 = HC2 = HC3 = HC4 = 0.) The mass burning function was taken to be the simple cosine burning function (CSBURN = T). It is the special case of the Fourier burning function (eqs. (I-92) to (I-97)) obtained with a zero relaxation parameter and only the first two Fourier coefficients nonzero. Any discontinuous changes of pressure during intake or exhaust are assumed to take place isentropically (eq. (I-118)) for case 512 (SP = T) and by a minimum internal energy expenditure for case 513 (HP = T).

Case input, excerpts from the printed output, and some plotted output are given in appendix D. This example does not require transport data because the Eichelberg heat transfer coefficient is being used and because the modeling levels are less than 4. The thermodynamic data are listed in appendix A and the chemical kinetic data in appendix C.

Appendix D contains case input and examples of some printed output for cases 512 (KASE = 512) and 513 (KASE = 513). For case 512 this output includes input information and excerpts of intermediate output (DEBUG = T) for ideal cycle 1 (level 1), nonideal cycle 1 (level 2), and nonideal cycle 4 (level 3). Also shown are cycle summary sheets for the converged ideal cycle (cycle 4, level 1) and several nonideal cycles (cycles 1 to 3, level 2; and cycle 8, level 3). The appendix also gives computer-drawn plots of a number of calculated quantities for nonideal cycles 3 and 8.

These results demonstrate the obvious fact that heat transfer will generally have a substantial effect on the calculated quantities (compare level 1, cycle 4, with level 2, cycle 3). Equally clear is the fact that, for this example, burned-gas kinetics (level 3) causes relatively small changes in temperatures and pressures but significantly affects nitric oxide (NO) concentrations (compare nonideal cycles 3 and 8).

Appendix D also displays cycle summary sheets (level 1, cycle 4; level 2, cycle 3; and level 3, cycle 8) and four plots for case 513. A comparison of cases 512 and 513 shows that the differences between the two are not major and are perhaps most easily discernible in the temperature and NO concentrations.

The calculation times for a cycle are shown at the bottom of the cycle summary sheets. For cases 512 and 513 these times are less than or equal to 1/4 second for level 1, 3¼ seconds for level 2, and 7 seconds for level 3. These values will change somewhat as problem conditions are altered, as will be seen in some of the other examples, but they may be regarded as reasonably typical times. On an IBM 360/67 the times would be about 14 times longer, but on a CRAY 1S they are shorter by a factor of 5.

Example II (Cases 1359 and 13591; Levels 1, 2, and 4)

Case 1359 is another example of the lean combustion of a hydrocarbon mixture (EQRAT = 0.9) with a fuel mixture of n-octane (C_8H_{18}), toluene (C_7H_8), benzene (C_6H_6), and 1-octene (C_8H_{16}). The oxidizer is now dry air (RHUMID = 0), the fuel is fully vaporized, and the fresh charge to the engine contains 10 percent recirculated exhaust gas (EGR = 0.1). Although the heat transfer coefficient is again of Eichelberg form and the mass burning function is the same as in example I, the burning interval (THBURN) is now considerably shorter. The two significant new features of the problem, in addition to exhaust gas recirculation, are supercharging (manifold pressure exceeds exhaust pressure, PMFOLD = 2 and PEXH = 1) and valve timing. The exponential form of the expression for $l^{(\pm)}/d$ (eq. (I-117b)) is used to calculate valve lift (FLOWIN namelist).

Appendix E gives the case input for this example along with some printed and plotted output. Level 4 calculations require shear viscosity data for pure gaseous species (appendix B) and gas-phase chemical kinetic data (appendix C) for the burned gas. The printed output includes cycle summary sheets for all three modeling levels (level 1, cycle 5; level 2, cycle 4; and level 4, cycle 6). Appendix E also shows plots of the indicator diagram, the temperature, and the CO and NO concentration and mass for cycles 4 and 6. The inclusion of valve timing has a substantial effect on all quantities except CO concentration.

The calculations for case 1359 were repeated with all input unchanged except for the program variables ALFAIN and ALFAEX, in namelist FLOWIN, which were set to their default values. The resulting calculations were designated as case 13591. Appendix E contains a cycle summary sheet and plots of the indicator diagram and mass for cycle 6. A comparison with the corresponding cycle of case 1359 shows a considerable diminution of the pumping loop.

Calculation times for levels 1 and 2 are comparable to those for example I. Level 4 calculation times are less than 15 seconds per cycle.

Example III (Case 99; Levels 1, 2, and 4)

Here we have an illustration of calculations for a motored engine (THBURN = 0), that is, one in which no chemical reactions take place because of the absence of a spark. The fresh charge to the engine is a mixture of gaseous propane and humid air (RHUMID = 75). The formula for the heat transfer coefficient (eq. (I-105)) is now chosen as the Dittus-Boelter form (HC2 = 0.3872, HA = 0.4, and HB = 0.8), and valve lift is calculated with the polynomial form for $l^{(\pm)}/d$ (eq. (I-117b))(POLY = T). In appendix F we give cycle summaries for ideal cycle 11 and two nonideal cycles (level 2, cycle 4; and level 4, cycle 8). For these nonideal cycles we also show plots of the indicator diagram, heat loss, and mass.

There are several features of the results which should be pointed out. For example, this is the first instance of a problem where a substantial quantity of mass is added to the working fluid by reverse flow through the exhaust system. This happens for all three modeling levels. Also this is the first time that the intake flow equations of the first specialization model break down as discussed in Chapter I at the end of the section First Specialization – Simplified Intake and Exhaust. This can be observed by the behavior of the heat loss rate at $\theta = 180°$ for cycle 4. Finally there is a substantial difference in the behavior of the pumping loops on the indicator diagrams for cycles 4 and 8. It should also be observed that the pressure during the power stroke is lower than that on the compression stroke for both indicator diagrams. This is caused by heat losses.

Example IV (Case 111; Levels 1, 2, and 5)

This example is a rich combustion (EQRAT = 1.25) of gaseous propane by humid air accompanied by exhaust gas recirculation. The mass burning function is of the Wiebe type, eqs. (I-99) to (I-102)(BETA = 3.2, TAU = 8.93E-05). In addition to the choice of burning function this problem offers the first appearance of level 5 modeling (KFLAME = 3). That is, a full kinetic treatment of the combustion of propane which uses a mechanism with 121 reactions (appendix C).

The calculations show some rather bizarre behavior as is evident from the information in appendix G. There we have assembled the cycle summary sheets for ideal cycle 6 (level 1); level 2, cycle 2; and level 5, cycles 11 to 15, as well as plots of the indicator diagram, the temperature, the CO concentration, and the mass for cycles 11 to 15. We have also included a plot of the Wiebe function for level 2, cycle 2. It corresponds to the curve for the burned mass fraction shown in the first plot for Case 111. Perhaps the most amazing feature is the fire-misfire behavior shown by cycles 11 to 15. It shows a periodic behavior with a period of four cycles, as can be seen by comparing cycle 11 with cycle 15, and manifests itself as early as cycle 4. It is caused by the too rapid injection of unburned gas into the burned gas. Since the initial pyrolysis reaction of hydrocarbons is endothermic, this serves to quench the reaction before it reaches the exothermic stage. This quenching effect plus the subsequent exothermic reaction is clearly demonstrated in the temperatures for cycles 11, 14, and 15. Obviously chemical kinetics sets an upper limit to the mass burning rate because this kind of behavior is never observed with equilibrium flames. Equilibrium flames release much of the energy instantaneously. This quenching phenomenon, perhaps occasioned by charge distribution nonuniformities, might be responsible for some of the cycle-to-cycle variation observed in real engine data.

Within each four-cycle period there is a great difference in behavior from cycle to cycle. It is particularly interesting that the indicator diagram does not close on cycles 12 to 14 and is indicative of nonsteady behavior within the period although the behavior may be considered to be steady from period to period.

As can be seen from cycle summary sheets, the computation times at level 5 are of the order of 1 minute or less.

Example V (Case 10; Levels 1 and 2)

For better than 99.9 percent of all problems, air will be the oxidizer of choice. The computer program reflects this bias toward air by building it into the program as a standard oxidizer so that only fuels need be specified. Yet occasionally one might want to use some other oxidizer. The primary purpose of this example is to illustrate how that can be accomplished. A secondary purpose is to show an alternative output format for compositions, which is advantageous when one is interested in the concentrations of trace species in the working fluid. Case input and a part of the output are given in appendix H.

The "fuel" in this example is a mixture of gases (NH_3, N_2, O_2, Ar, and CO_2) containing the oxidizer O_2. The "built in" oxidizer, air, is effectively suppressed by setting $A/F = 1 \times 10^{-5}$ (AF = 0.00001). It could equally well have been accomplished by assigning the percentage of fuel by weight (FPCT) to be nearly 100 percent. The air cannot be totally suppressed by using $A/F = 0$ (or

100 percent fuel) because this creates internal program difficulties. The gases N_2, O_2, Ar, and CO_2 in the "fuel" are in the same proportions as in ordinary air. The relative amounts of NH_3 and O_2 are in stoichiometric proportions. Appendix H gives cycle summary sheets for ideal cycle 5 (level 1) and for cycle 5 (level 2).

With levels 1 and 2 and the Eichelberg heat transfer coefficients, no transport or chemical kinetics data need be included in the input.

Example VI (Case 222; Levels 1, 2, and 5)

Example VI differs from example IV in only a few particulars. The recirculated exhaust gas has been reduced from 10 percent to 5 percent; the humid air has been changed to dry air. Finally the form of the mass burning function is now the Fourier burning function with coefficients chosen to retard the initial burning rate to avoid quenching the reaction (AN = 0.375, −0.5, and 0.125). The burning function is, in fact, one of those illustrated in figure 5 of Chapter I. The purpose of this example is to illustrate the program's restart capabilities and its ability to accommodate cycle-to-cycle variation in some of the parameters of the problem. We shall confine our parameter variation to the air-fuel weight ratio to demonstrate the rather significant effect that air-fuel variations can have on cycle-averaged exhaust gas compositions. Case input and a part of the output are given in appendix I.

Our plan is to run an adequate number of level 5 cycles at a stoichiometric air-fuel ratio to reach steady state conditions. At that point we will begin to vary the air-fuel ratio by random picks from a suitable distribution function, with stoichiometric mean, and continue the cycle calculations until we have calculated 25 exhaust gas compositions which are affected by the air-fuel ratio variation. At that point a comparison of the steady state composition with the average of the 25 variable cycles will show the effect of the random variations.

For our distribution function we have chosen a Pearson type III distribution (ref. 3), which is nothing more than a transformed χ^2 distribution. It is a three-parameter distribution function with parameters γ, p/a, and $p+1$. The (cumulative) distribution function $F(x;\ \gamma,\ p/a,\ p+1)$, the frequency function $f(x;\ \gamma,\ p/a,\ p+1)$, and the moment-generating function $M(\theta;\ \gamma,\ p/a,\ p+1)$ are given by

$$F(x;\gamma,p/a,p+1)\equiv\frac{1}{\Gamma(p+1)}\int_0^{(x-\gamma)p/a} dy\ y^p e^{-y} \qquad \gamma\le x\le\infty$$

$$f(x;\gamma,p/a,p+1)\equiv\frac{\partial F}{\partial x}=\frac{(p/a)}{\Gamma(p+1)}y^p e^{-y}\bigg|_{y=(x-\gamma)p/a} \qquad \gamma\le x\le\infty$$

$$M(\theta;\gamma,p/a,p+1)\equiv\int_\gamma^\infty e^{\theta x}f\,dx=e^{\theta\gamma}(1-\theta a/p)^{-(p+1)}$$

where $\Gamma(p+1)$ is the usual gamma function. The parameters are not completely arbitrary and must satisfy γ real and finite, $p+1\neq -k$, where $k=0,\ 1,\ 2,\ \ldots$, and $p/a>0$. The cumulants κ_i of the distribution are expressible in terms of the parameters of the distribution.

$$\kappa_1=\gamma+(p+1)\frac{a}{p}$$

$$\kappa_i=(i-1)!(p+1)\left(\frac{a}{p}\right)^i \qquad i=2,\ 3,\ \ldots$$

The first cumulant is the population mean, and the second and third cumulants are identical to the second and third moments about the mean.

The k statistics are sample estimates of the cumulants and are expressible in terms of the sample mean m_1 and moments about the mean m_k, where $k = 2, 3, \ldots$ For a sample of size N

$$m_1 = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$m_k = \frac{1}{N} \sum_{i=1}^{N} (x_i - m_1)^k \qquad k = 2, 3, \ldots$$

and these are used together with the relations

$$k_1 = m_1, \quad k_2 = \frac{N m_2}{N-1}, \quad k_3 = \frac{N^2 m_3}{(N-1)(N-2)}, \quad k_4 = \frac{N^2\left[(N+1)m_4 - 3(N-1)m_2^2\right]}{(N-1)(N-2)(N-3)}$$

to give the first four k statistics. We selected $\gamma = 10.6787$, $p/a = 1.2$, and $p + 1 = 6$ as our parameter values. We chose two random samples from the distribution function with these parameters: one of size $N = 5000$, and the other of size $N = 25$. The larger sample was used to test the correctness of our method of picking a sample and the smaller sample was used in the cycle calculations. Table VIII shows the results. The first cumulant κ_i is the stoichiometric air-fuel ratio for the combustion of propane by dry air. The second cumulant implies a spread about the mean of about two units. This corresponds to an equivalence ratio varying from about 0.8 to 1.25. From the table it is clear that k statistics for $N = 5000$ are an excellent approximation to the population cumulants. The $N = 25$ sample is slightly to the rich side of the stoichiometric air-fuel ratio with a somewhat smaller spread about its mean.

The results of the calculation for case 222 are summarized in appendix I, where we present cycle summary sheets for ideal cycle 5 (level 1), nonideal cycle 3 (level 2), and nonideal cycles 4 to 37, which are level 5 calculations. The air-fuel ratio remains stoichiometric through nonideal cycle 11 and begins its random variation on cycle 12 (actually at the end of cycle 11, where the intake valve opens). The resultant variation in composite exhaust gas properties is first detected on cycle 13 although the composite exhaust gas properties have been slightly affected during valve overlap early in cycle 12. The cycle summary sheets show that the operation is effectively at steady state between nonideal cycles 7 to 11 except for minor cycle-to-cycle variations.

Appendix I shows plots of the indicator diagram, the temperature, CO and NO concentrations, the mass burning function, and the cycle mass for cycle 11 as indicative of steady state, stoichiometric operation. The significant effect of variations of the air-fuel ratio on cycle operations can be seen by comparing CO and NO concentrations for cycle 11 with those shown in similar plots for nonideal cycles 12, 17, 22, 27, and 32. Tables IX and X compare cycle-averaged, composite exhaust gas properties for the six steady state nonideal (stoichiometric) cycles 7 to 12 and the 25 nonideal cycles 13 to 37 with varying air-fuel ratio. It is obvious that moderate cycle-to-cycle variations in air-fuel ratio can have a dramatic effect on cycle-averaged exhaust gas compositions. Observe that carbon monoxide concentrations are increased by a factor of almost 15 and hydrocarbons, absent for the constant, stoichiometric air-fuel ratio results, are present at a concentration in excess of 300 ppm by mass when the air-fuel ratio varies about the stoichiometric value. The effect on other quantities, while important, is considerably smaller.

This example was run with three restarts as shown in the input in appendix I. The initial run had 10 nonideal cycles. The first three were level 2, and the remaining seven were level 5 (KFLAME = 4). Level 5 calculations require both transport data and a chemical kinetic mechanism for the fuels and the products (appendix C). Also required is a FLOWIN namelist which follows the AFINP namelist with KFLAME = 4 in the case input. The first 10 air-fuel mixtures are stoichiometric (EQRAT = 1). For the restarts the mixtures are the result of random picks from the Pearson type III distribution mentioned previously. The k statistics for the random sample are those given in the column labeled $N = 25$ in table VIII.

Description of Computer Program

General Comments

The computer program ZMOTTO is very complex, containing over 70 routines. It is written in standard Fortran IV and was tested on the IBM 370/3033, the IBM 360/67, and the CRAY 1S computers. In developing ZMOTTO we have always placed the emphasis on safety and accuracy rather than on mere computational speed. To construct ZMOTTO we have used, and considerably revised, portions of two existing computer programs. The first is Gordon and McBride's computer program CEC (ref. 1) for thermodynamic computations, and the second is Hindmarsh's program GEAR (ref. 4) for numerical integration of ordinary differential equations. The extent of our revisions is spelled out in the description of the various subroutines.

Because of the number and complexity of the individual subroutines it is virtually impossible to discuss them in any detail. In our verbal discussion of the routines we have attempted to refer to the appropriate equations of Chapters I to III in order to help the interested reader in deciphering the contents of a particular routine. Also we shall give three flow charts to convey the overall organization of ZMOTTO.

Some of the program subroutines have multiple entry points. Most of these entry points are actually independent routines, with no shared programming, that have been collected in a subroutine only to share many sets of labeled COMMON. There are only five entry points (CHARGE, CB2, CB3, CONTNU, and VONLY), which break into routines to share portions of the programming.

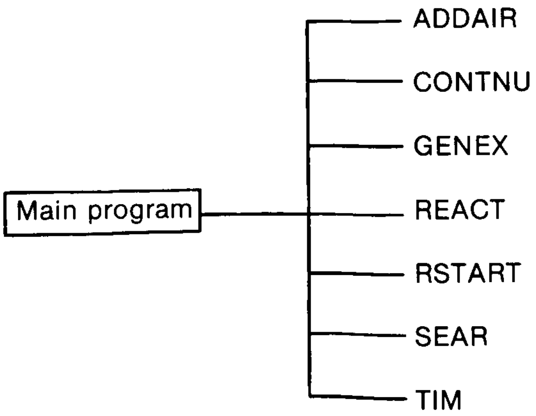
Subroutines and subroutine entries are listed in table XI, which organizes them by modeling level. Routines which appear in the first column are used for levels 1 to 5. Those in the second column contribute to levels 2 to 5, and so on. Subroutine entries are identified by listing the subroutine name in parentheses following the entry name. In each column the routines have been loosely organized into several categories according to their purpose. Routines under the executive category play a major role in the flow of the program. Some routines are listed in more than one category.

The main executive routines are the main program and a large subroutine GENEX. The main program directs the flow according to whether a computer run is an initial run or a restart run. GENEX directs the cycle-to-cycle program flow for all levels. Flow charts for these two routines and a diagram showing the general flow among the principal routines involved with burning for the nonideal cycles are given in appendix J.

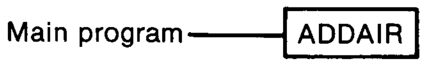
Brief descriptions of each routine and BLOCK DATA are given in the following paragraphs, where they appear in alphabetical order except for the main program, which is given first. A brief diagram is given at the end of each description. In the diagram any routines calling the routine being described are shown to its left, and any routines called by the routine appear on its right.

Synopses of Individual Routines

Main program. – The main program reads some of the case input and directs program flow according to the codes REAC, OMIT, NAME, and RESTART on the input cards (table II). A flow chart of this routine is given in appendix J.

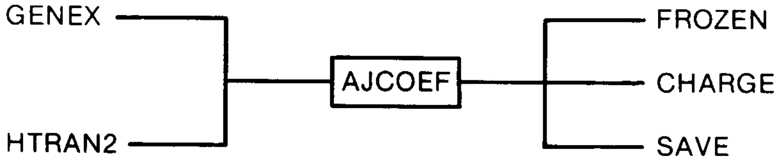


ADDAIR (add air). – ADDAIR is an entry in subroutine AJCOEF. It adds air to the list of reactants by setting variables for the oxidant air that are similar to variables which have been set by subroutine REACT for the fuels.

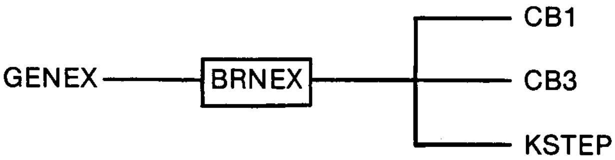


AIRSET (air set). – AIRSET is an entry in subroutine AJCOEF. It combines the coefficients for the thermodynamic data of N_2, O_2, Ar, CO_2, and H_2O (if $RHUMID \neq 0$), by averaging over the air composition, into a set of coefficients for air. These coefficients are stored in the COEF array after the coefficients for the fuels. Air data are indexed as JAIR. The coefficients are also stored in the COEF set indexed as NS1 = JAIR + 1. The NS1 coefficients are adjusted later in AJCOEF to represent the unburned working fluid as required.

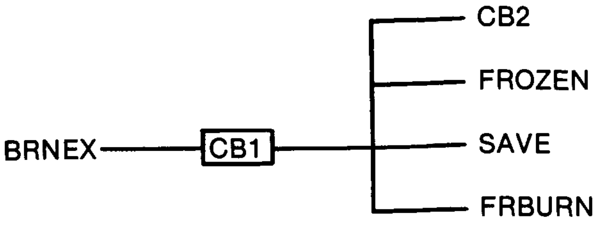
AJCOEF (adjust coefficients). – The program subroutine AJCOEF contains many entries. All entries are discussed separately. The value of EM (i.e., ratio of mass of charge to mass of residual exhaust gas) is calculated according to equations (III-51) to (III-56), (III-90), and (III-91) for levels 1 to 3. By using EM, a set of thermodynamic coefficients COEF are calculated to represent the properties of the unreacted working fluid. For the ideal cycle, EM is used to obtain station 3 properties (column 3 in the output). EM is obtained iteratively with a maximum of 10 iterations. Station 2 properties for supercharge cases (i.e., PMFOLD > PEXH) for levels 1 to 3 are obtained in a similar way. For level 3 calculations, EM is used to obtain properties of the cylinder contents at points intermediate to stations 2 and 3.



BRNEX (burning executive). – BRNEX is an executive routine for finite-rate burning which takes place between stations 4 and 5 for levels greater than 1. A sketch of the program flow for finite-rate burning is given in appendix J. For cycles without chemical kinetics (level 2), BRNEX calls CB1 at the start of burning, and control is returned to BRNEX at the completion of burning. For levels greater than 2, CB1 is called once for initial calculations. Flow then goes to entry CB2, where estimates for intermediate output points for printing and plotting are calculated along with other calculations. Thereafter DIFEQ calls CB2, and BRNEX calls KSTEP for chemical kinetic calculations between the output points. Except for special points the actual output points are usually beyond the calculated output points. To avoid changing integration step sizes, the actual output point is the end of an integration step immediately following a calculated output point. CB3 completes the calculation of the properties for the actual output point.



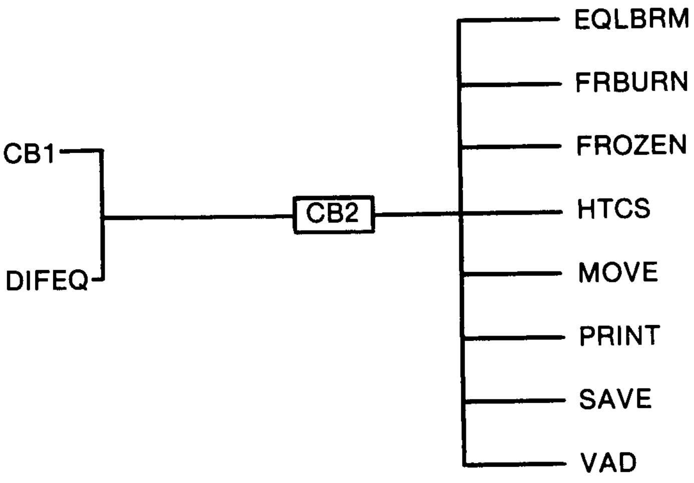
CB1 (combustion 1). – Subroutine CB1 and its two entries CB2 and CB3 comprise most of the finite-rate burning calculations which start at station 4 and end at station 5 for levels greater than 1. The flow of the program is indicated in appendix J. Subroutine CB1 includes initialization, calculation of station 4 properties, and calculation of the burning endpoint, station 5, as given by equations (III-31) to (III-34).



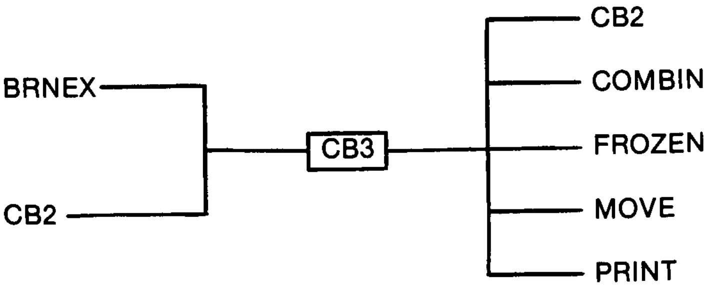
CB2 (combustion 2). – CB2 is an entry in the program subroutine CB1. It contains a major part of the finite-rate burning calculations. See appendix J for the program flow to and from CB2. For intermediate output and plotting, properties are calculated for both burned and unburned mixtures. For printed output, even-numbered columns 2 to 12 (indexed NPT1) are burned-gas properties. Odd-numbered columns 3 to 13 (indexed NPT) are unburned-gas properties.

For level 2 cycles, CB2 sets the step size and output points (eqs. (III-82) to (III-89)). It integrates equation (III-76) for the burned- and unburned-gas temperatures by using equations (III-78) to (III-80). See equation (III-81) for convergence criteria. For each temperature iteration (indexed ITU ≤ 7) there is an iteration to convergence on specific volume VLM (ITV ≤ 7).

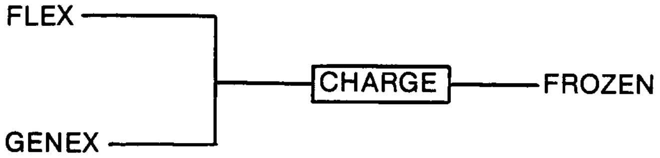
For levels greater than 2, the level 2 step-size calculations are used to estimate output points (see BRNEX). Some other calculations are used in the numerical integration, but no iterations occur in CB2 for these higher levels. After the first point, CB2 is called from DIFEQ.



CB3 (combustion 3). – CB3 is an entry in subroutine CB1. It completes the calculations at the intermediate output points during burning. See the writeup for CB2 and appendix J. At the end of combustion, what is left of the unburned gas is combined with the burned gas to form a single set of properties and composition for station 5.

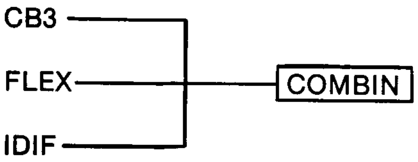


CHARGE (charge composition and properties). – CHARGE is an entry in AJCOEF. It calculates the composition and properties of the fresh charge to the cylinder including EGR and residual exhaust gas. Values are stored in arrays with index NPT = 1 (column 1 of the intermediate output).

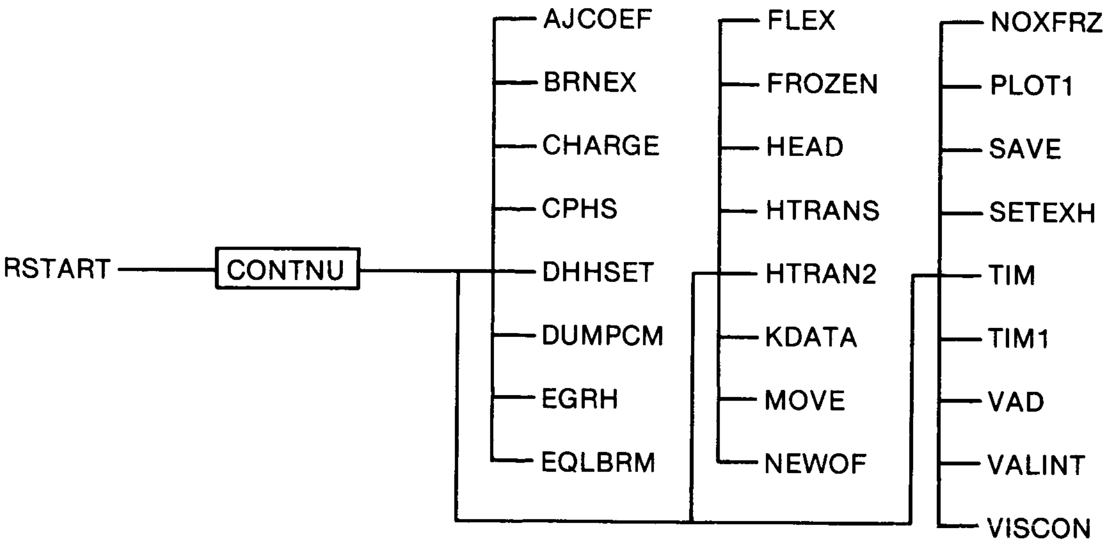


CLRY (clear Y). – CLRY is a short routine used to set the derivatives of some dependent variables to zero during numerical integration calculations for chemical kinetics and poppet valve flow (levels 4 and 5). It sets to zero the derivatives (1) for compositions after the intake valve closes (station 3) and (2) for mass after burning (station 5) if the exhaust valve has not opened.

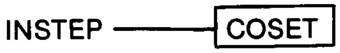
COMBIN (combine air and fuel with products). – COMBIN is an entry in AJCOEF. It combines the moles of air with the individual burned-gas constituent species. This is done at the end of combustion (called by CB3) for levels 2 to 4. For level 5, COMBIN also combines the moles of the individual fuels with the corresponding product species. This is done at the beginning of combustion (called by IDIF) and, when the exhaust valve closes (called by FLEX), for the composite exhaust gas.



CONTNU (continue). – CONTNU is an entry in GENEX. It is called from RSTART to continue cycle calculations either after some point given in the restart input or after the last cycle dumped during a previous computer run. Restarting can only take place at the beginning of a computational cycle for calculation levels greater than 1. See the flow chart of GENEX in appendix J for the program flow following entry CONTNU.

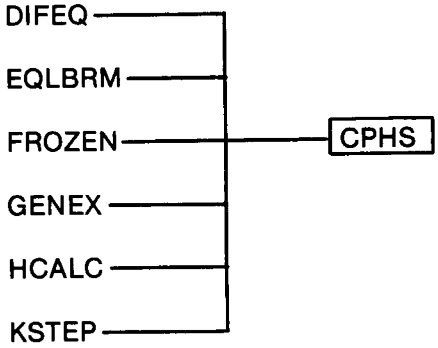


COSET (set coefficients). – This routine sets the coefficients used in the integration. It differs from Hindmarsh's routine COSET (ref. 4) only in the choice of some of the coefficients and the requirement that the maximum integration order be 8 or less. The integration coefficients are those discussed in Chapter II. See equations III-40 to III-43 of Chapter III and for additional details see Chapter II.

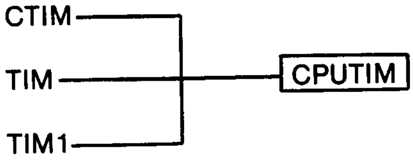


CPHS (calculate C_p, H, and S for species). – CPHS calculates thermodynamic properties for individual species at temperature TT by using the coefficients COEF. The empirical equations are given by equation (III-112) (where C_p is dH/dT in eq. (III-112)). Appendix A lists the coefficients used with the sample problems. The properties are calculated for all species with index between JS1 and NS.

For the COEF (i,j,k) array, i labels the seven coefficients, j labels the species, and k = 1 or 2 is for the temperature intervals. The value k = 1 is for the higher interval and k = 2, for the lower interval (1000 to 5000 K and 300 to 1000 K, respectively, in appendix A).

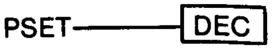


CPUTIM (central processing unit time). – CPUTIM is a user-supplied routine for the program ZMOTTO. At the NASA Lewis Research Center it gives the computer time in milliseconds. It is used to calculate (1) total program time, (2) cycle times, and (3) times between stations for levels greater than 1. If a CPUTIM routine is not provided, all times will be set to zero.

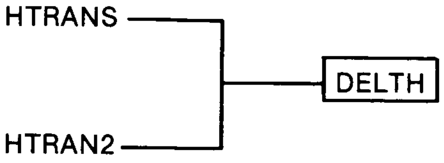


CTIM (cycle time). – CTIM is an entry in TIM. If a CPUTIM routine is provided, CTIM calculates cycle times to be printed at the end of each Otto cycle. If CPUTIM is not provided, all times will be set to zero.

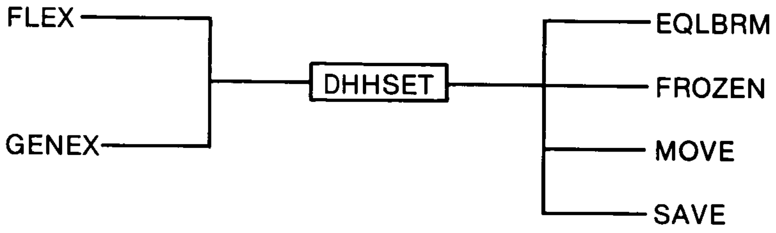
DEC (decomposition). – This routine is identical to Hindmarsh's routine DEC (ref. 4), which in turn is a slightly modified version of Moler's routine DECOMP (ref. 5). It is a matrix triangularization routine using Gaussian elimination with partial pivoting. The back solution is performed by subroutine SOL.



DELTH (delta theta). – DELTH is an entry in VAD. It is only used for levels 2 and 3. It is called from HTRANS and HTRAN2 for all parts of the cycle with two exceptions: it is never called during combustion (IPT = 5), and it is not called during postcombustion (IPT = 6) for level 3. It calculates step sizes DTH according to equations (III-73) and (III-74) and sets the next crankangle for intermediate output. It also calculates some other variables, including the derivatives given by equations (III-44), (III-47), and (III-48).



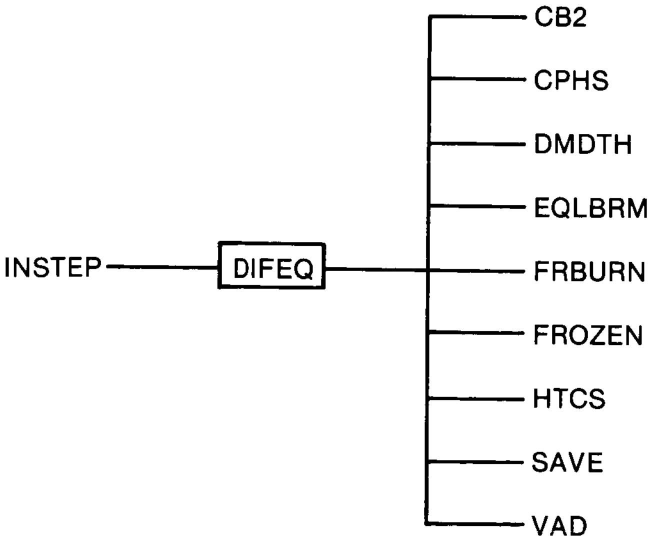
DHHSET (delta H set). – DHHSET, an entry in AJCOEF, calculates the enthalpy difference used in calculating the chemical energy (eq. (III-102)) required for several output parameters in OOUT.



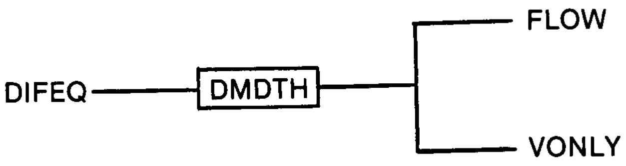
DIFEQ (differential equations). – DIFEQ is one of the routines required for finite rate chemistry. It calculates the vector $\dot{y}=f(y, t)$ in the form required by the numerical integration package. The program vector is YDOT. The equations for YDOT are given by (I-143) to (I-145), (III-1), and (III-2).

The first components of YDOT are for the species in the kinetic order (indexed 1 to LS). The kinetic order is the order of species as they are first encountered in the reaction mechanism. This order is set in subroutine KDATA and printed out before cycle calculations begin. These YDOT's are followed by the nonreacting species (indexed LS + 1 to NQS), temperature (indexed NQT), mass if level 4 or 5 (indexed NQM), and unburned-gas temperature during combustion (indexed LSP2). During combustion (INT = 2) the index NQT is used for the burned-gas temperature.

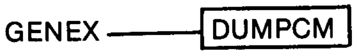
For equilibrium flames (ICYCLE < KFLAME, levels 3 and 4) and during combustion for level 2, the equilibrium temperature and composition are sometimes estimated by subroutine SAVE rather than calculated by subroutine EQLBRM and its associated routines. Estimates are determined in subroutine SAVE by using equations (III-29) and (III-30).



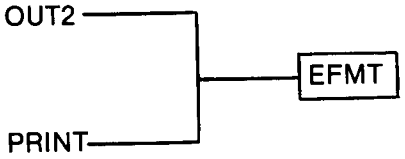
DMDTH (derivative of mass with respect to theta). - DMDTH calculates MDOT, the derivatives of mass with respect to crankangle for flow problems, levels 4 and 5. MDOT is indexed 1 for the intake valve and 2 for the exhaust valve. It is calculated by using equations (I-110) to (I-117) and (III-35) to (III-39). For flow into the cylinder MDOT is greater than zero. For flow out of the cylinder MDOT is less than zero. The properties and composition of incoming and outgoing gases are stored according to the index IG. IG = 1 for the fresh charge, IG = 14 for gas which previously left the cylinder through the intake valve, and IG = 15 for composite exhaust gas.



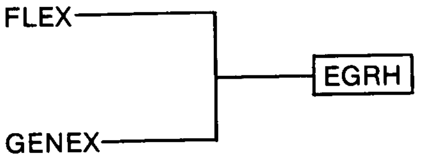
DUMPCM (dump COMMON). - At the end of each nonideal cycle (levels greater than 1) the contents of most of the labeled COMMON are copied by DUMPCM onto I/O unit 7 for restarting and plotting.



EFMT (E format). - EFMT is used to print numbers in a compact exponential form similar to the Fortran E format. It is used for mole fractions with the TRACE option and density. It is used for level 1 calculations and intermediate output for the higher levels.

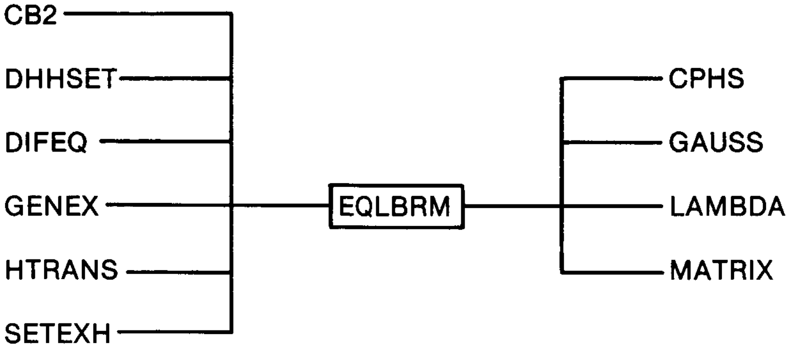


EGRH (enthalpy of recirculated exhaust). - EGRH is an entry in AJCOEF. It calculates the enthalpy of the recirculated exhaust gas, HEGR, to be used in calculating the properties of the charge in the CHARGE routine, which is also an entry in AJCOEF. See Chapter III, the section Fresh Charge Specification for a further discussion of the exhaust gas properties.



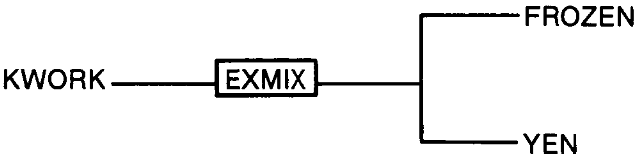
EQLBRM (equilibrium). - EQLBRM is the core routine for the equilibrium calculations. It calculates compositions and thermodynamic properties indexed NPT. The routine is similar to the subroutine of the same name in the Gordon-McBride CEC program (ref. 1) but has two major changes. First, the components are updated at every point to be the most abundant set of species describing the chemical systems. This is checked near convergence or sooner if a singularity occurs. For the latter case the number of components may be reduced in order to obtain an independent set of equations. Generally this change will result in more accuracy and solve more problems. The old EQLBRM used the atomic elements as components. Second, instead of using initial estimates to be the values from a previous calculation directly, the values are corrected by using the thermodynamic derivatives given by equations (III-29) and (III-30). These estimates are calculated in subroutine SAVE.

The control factor AMBDA for the corrections during the iteration procedure in EQLBRM is now calculated in a separate routine LAMBDA since it is also used by the SAVE routine. The IONS option has been removed for this program. See table XII for the assigned state variables required for each call to EQLBRM.



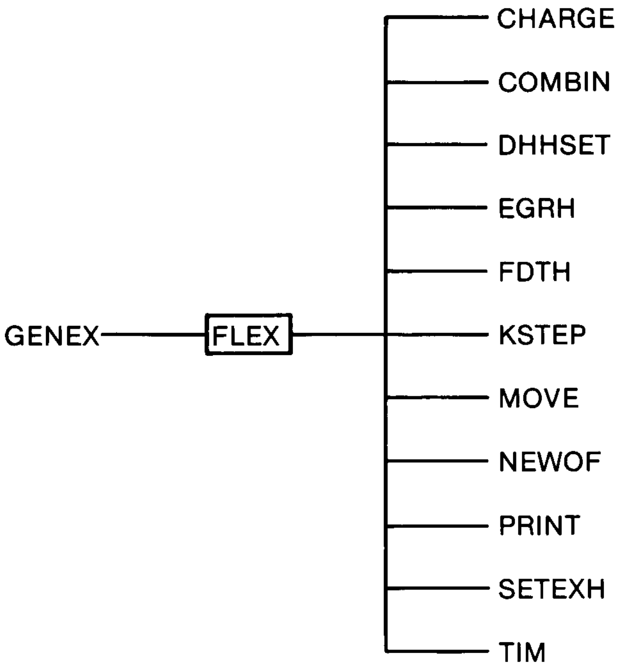
EXMIX (exhaust mixture). – EXMIX is used for levels 4 and 5 to calculate the mass, enthalpy, and composition of gas mixtures which have left the cylinder through the intake and exhaust valves. The routine is called at the end of each numerical integration step. If there is outflow (i.e, if the current pressure is greater than the manifold pressure for the intake valve or greater than the exhaust pressure for the exhaust valve), quadrature formulas are used to integrate values of mass, composition, and enthalpy of the exhaust mixture. The formulas are given by equations (I-121), (I-122), (III-15) to (III-19), (III-22), and (III-23). For inflow, integration continues for mass alone until all the mass which has escaped has been returned to the cylinder. This mass, TMASS, is a negative value until the point where it has all returned; then TMASS = 0.

Extrapolation formulas ((III-12) to (III-14)) are used to predict the points where the pressure is expected to equal the manifold or exhaust pressure and where TMASS = 0. At the appropriate points these predictions are used to temporarily adjust the numerical integration step to hit these points exactly.

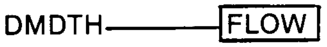


FDTH (flow delta theta). – FDTH is used with levels 4 and 5 to set approximate points for intermediate output and plotting for all parts of the cycle except combustion. Except for station points and some other selected points the interval is set to 5 crankangle degrees in FDTH. However, the actual point will normally be beyond the 5° step so that the output point is actually the end of an integration step. This avoids both changing integration step sizes and interpolation.

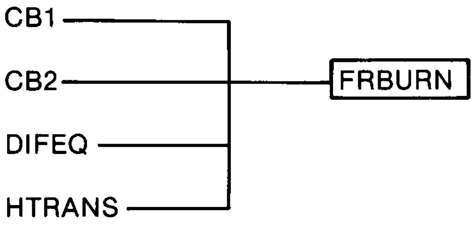
FLEX (flow executive). – Subroutines FLEX and GENEX are the executive routines required for cycles with poppet valve flow, levels 4 and 5. GENEX calls FLEX to do various portions of these higher level cycles except for combustion, which is directed by BRNEX. The flow chart for subroutine GENEX in appendix J shows the program flow among these three routines. FLEX calls KSTEP for numerical integration between output points.



FLOW (flow functions). – Subroutine FLOW evaluates the poppet valve flow functions given in equations (I-117a) and (I-117b).

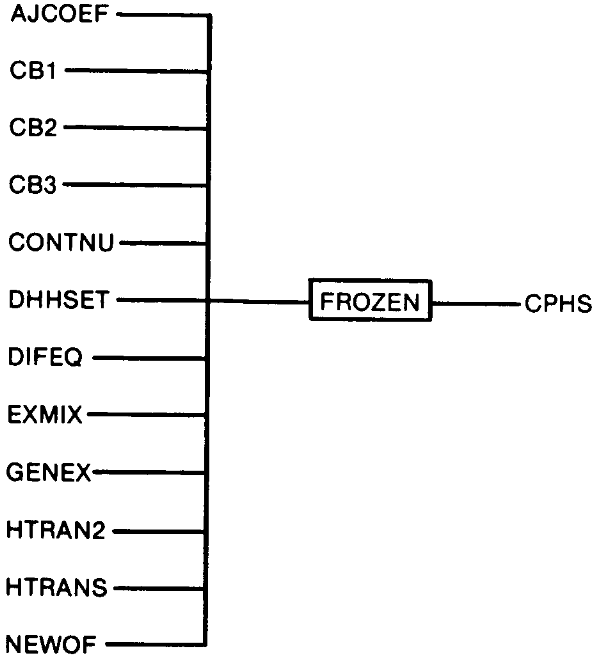


FRBURN (fraction burned). – Subroutine FRBURN calculates the mass fraction of burned gas according to the burning function indicated in the input and by using equations (I-92) to (I-104).



FROZEN (frozen compositions). – Subroutine FROZEN calculates thermodynamic properties for assigned thermodynamic states and the nonreacting compositions stored in EN(i, NFZ), where i is a species index. The assigned state variables are similar to the assignments required by the EQLBRM subroutine. They are summarized in table XII. The resulting properties are stored in arrays indexed NPT. NFZ may be equal to NPT. The routine is similar to the routine of the same name in the Gordon-McBride CEC program (ref. 1).

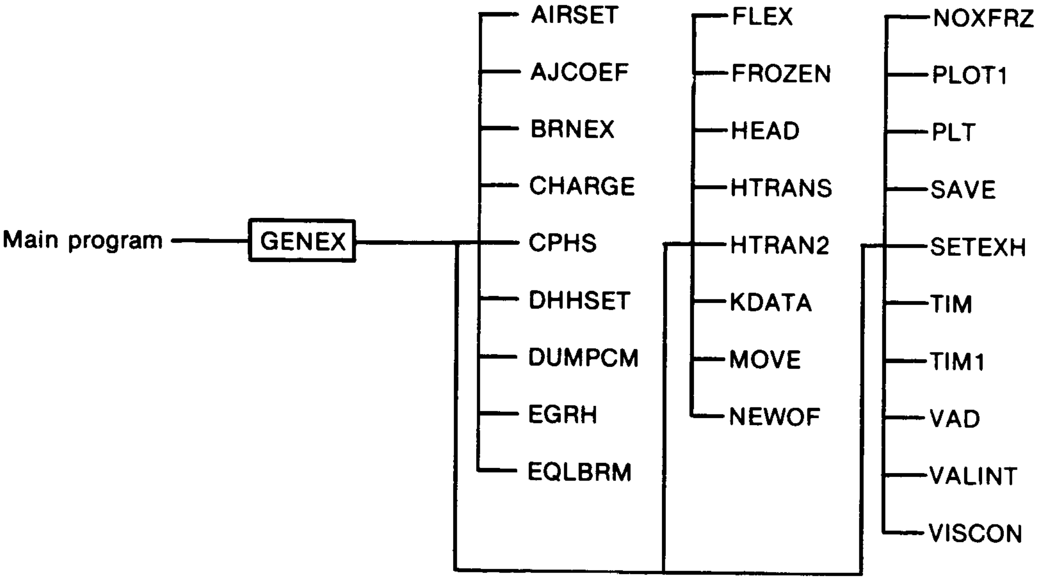
For assigned temperature problems no iteration is required. Otherwise there is an iteration on temperature until the desired assigned value of either enthalpy, internal energy, or entropy is obtained for a particular pressure or specific volume.



GAUSS (Gaussian elimination). – GAUSS is used to solve the set of simultaneous linear iteration equations constructed by subroutine MATRIX. The solution is effected by performing a Gauss reduction with a modified pivot technique. The routine is very similar to the routine of the same name in reference 1. The solution vector is stored in X(k).

GENEX (general executive). – Subroutine GENEX is the main executive routine for the program. An abbreviated flow chart for the routine is shown in appendix J. Generally it

(1) Initializes most of the variables
(2) Performs many of the initial calculations or calls routines that do
(3) Reads in the thermodynamic data for the fuels
(4) Reads and processes variables in OTTINP and AFINP namelists
(5) Controls miscellaneous calculations between successive cycles for all levels



HCALC (H calculations). – HCALC calculates enthalpies (H values) of the individual fuels, the total fuel, and air for the temperatures on the input cards. The routine is similar to the routine of the same name in reference 1. The routine is called once preceding the first ideal cycle.

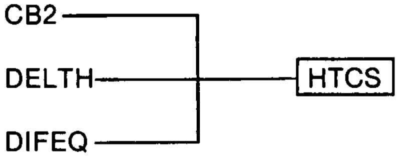
HEAD (headings). – HEAD is an entry to a routine in OOUT which prints headings and performance parameters for the summary sheets for all levels.

HTCS (heat transfer coefficients). – HTCS calculates the heat transfer coefficient HBAR by using equation (I-105).

If the Eichelberg form of the heat transfer coefficient is used (i.e., HC2 = HC3 = 0), HBAR is calculated as a function of temperature TK and pressure PK. However, if HC2 is not zero, transport properties of the individual species (eq. (III-113)) and the mixture (eqs. (I-152) and (I-153)) are calculated. The compositions are stored in EN (i, IK) for nonkinetic calculations and in Y0(j) for kinetic calculations, where i and j index the species.

If j is the species index for transport properties (maximum 30), some arrays are defined as follows:

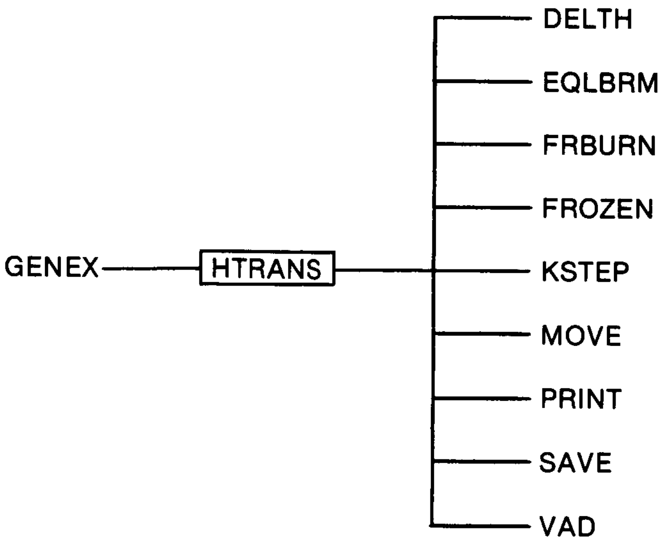
VTC (i, j, 1)	empirical coefficients (indexed i) for viscosity
VTC (i, j, 2)	empirical coefficients (indexed i) for thermal conductivity
VCSP (j, 1)	viscosity of the individual species
VCSP (j, 2)	thermal conductivity of the individual species
ICV (j)	index of the corresponding species in the thermodynamic data order
KCV (j, 1)	index of the corresponding species in the thermodynamic data order excluding condensed species
KCV (j, 2)	index of the corresponding species in the chemical kinetic data order



HTRANS (heat transfer). – HTRANS directs level 2 and 3 calculations between stations 1 and 2 (IPT = 2), 3 and 4 (IPT = 4), and 5 and 6 (IPT = 6). Generally many intermediate points are calculated for intermediate output and plotting.

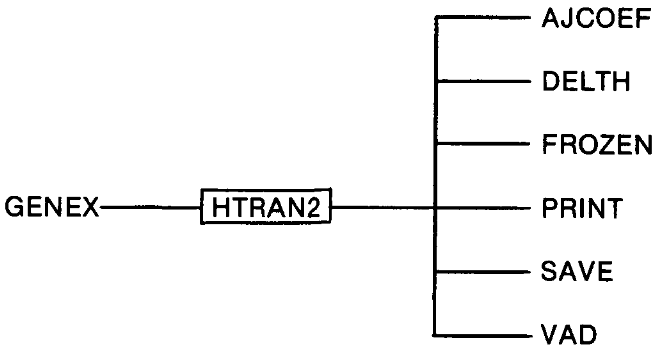
The integration methods are detailed in equations (III-69) to (III-72). Internal energy U(i) and volume VLM(i) are assigned to each point i for level 2 cycles (HP and VOL are true). For IPT = 2 or 4 the composition is frozen, and FROZEN is called to calculate the properties. For IPT = 6 and level 2 cycles, EQLBRM is called to calculate the properties.

For level 3 cycles (IPT = 6 only), KSTEP is called for integration calculations between print points. When station 6 has been reached and there still remains some unburned gas, FRBURN is called to obtain the mass fraction of the burned gas RBG.

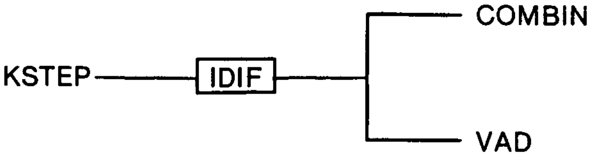


HTRAN2 (heat transfer 2). – HTRAN2 is an entry in subroutine HTRANS. It directs calculations for levels 2 and 3 between stations 2 and 3 (IPT = 3) and 7 and 8 (IPT = 8). Output points are determined by the DELTH routine for intermediate output and plotting. The integration methods are detailed in equations (III-69) to (III-72).

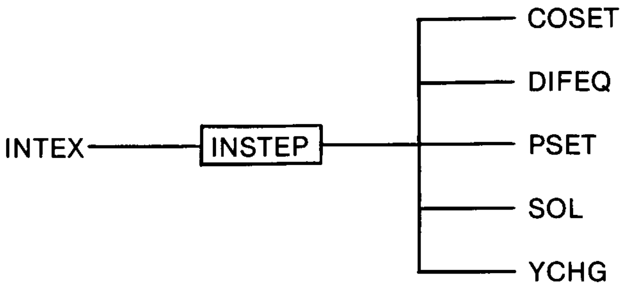
For calculations between stations 2 and 3 addition of the charge is required. These adjustments are done in subroutine AJCOEF. FROZEN is called in AJCOEF for assigned temperature and pressure (TP). Pressure is the manifold pressure (PP = PMFOLD). Temperature comes from density (RTH = 1/VLM (NPT)) and the ideal-gas equation of state. There is an iteration on density in HTRAN2. For calculations between stations 7 and 8 the composition is frozen. FROZEN is called with an assigned enthalpy (HSUB0) and pressure (PP = PEXH). There is an iteration on HSUB0.



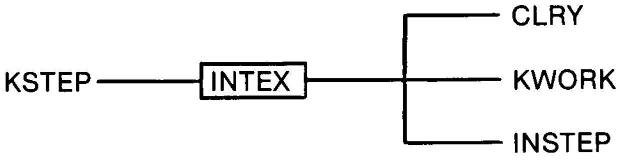
IDIF (initialize DIFEQ). – IDIF is an entry in DIFEQ which initializes the variables in DIFEQ.



INSTEP (integration step). – The routine INSTEP carries out one integration step, estimates truncation and integration errors, and selects step size and integration order. It is a drastic revision of Hindmarsh's routine STIFF (ref. 4). The theory of the method is described in Chapter II, in particular, the sections Some Special Cases and Step Size and Order Changes. Additional information is given in Chapter III in the discussion of integration methods for the general model. While the details of the computations performed in INSTEP differ radically from those of STIFF, its organization remains similar.



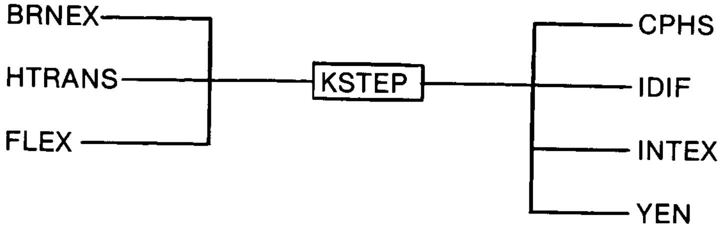
INTEX (integration executive). – This is an executive routine for the numerical integration package in ZMOTTO. The integration techniques are based on the analysis of Chapter II. INTEX differs from Hindmarsh's routine DRIVE (ref. 4) chiefly in three respects. Interpolation to desired output points has been eliminated, the capability of increasing the number of differential equations has been added, and some cycle-relevant calculations have been incorporated.



JACOB (Jacobian). – Subroutine JACOB calculates the Jacobian matrix for the numerical integration (see eqs. (II-37) to (II-41) and the associated discussion for some details). It is used during combustion and postcombustion for level 3 and throughout the cycle for levels 4 and 5. The elements are calculated by using equations (I-146) to (I-151) and (III-4) to (III-11).

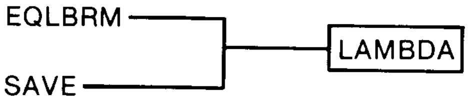
KDATA (kinetic data). – Subroutine KDATA reads the chemical kinetic data from I/O unit 9 as detailed in appendix C. Data are stored in arrays for use with numerical integration routines DIFEQ and JACOB.

KSTEP (kinetic step). – Subroutine KSTEP is the interface between the numerical integration routines and the remainder of the program. It is called at intermediate output points. For level 3 calculations, KSTEP is called from BRNEX during burning (IPT = 5) and from HTRANS during postcombustion (IPT = 6). For levels 4 and 5, KSTEP is called from BRNEX during burning and from FLEX for all other parts of the cycle. KSTEP calls INTEX for integration. After returning from INTEX, data are placed in arrays indexed by NPT for printing and plotting.

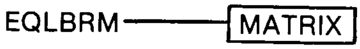


KWORK (kinetic work). – KWORK is an entry in DIFEQ. It is called from INTEX at the end of each numerical integration step. It calculates heat loss and work and keeps a running total of these values for intermediate output points. For levels 4 and 5 it calls EXMIX to keep track of mixtures which have exited through the valves.

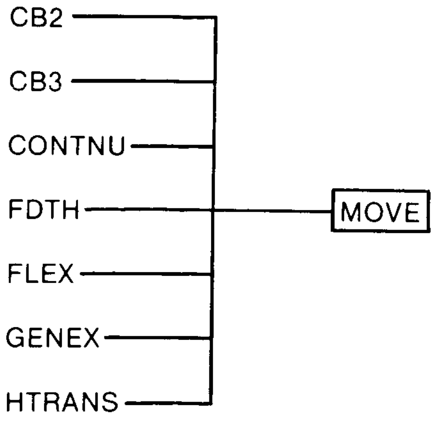
LAMBDA (lambda). – Subroutine LAMBDA calculates a control factor AMBDA which limits the size of corrections during the process of obtaining equilibrium compositions and temperatures. It limits the corrections calculated during the Newton-Raphson iterations in EQLBRM and also the estimated corrections calculated in SAVE by using equations (III-29) and (III-30). LAMBDA also applies the corrections. These calculations were part of the EQLBRM routine in the CEC program (ref. 1).



MATRIX (matrix). – Subroutine MATRIX sets up the matrices to solve for chemical equilibrium compositions and thermodynamic derivatives. The routine is essentially the same as the routine of the same name in reference 1.



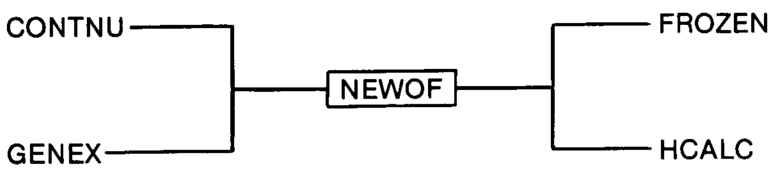
MOVE (move data). – MOVE is an entry in VAD which simply copies properties and compositions from arrays indexed ISV to arrays indexed NPT.



NEWOF (new air-fuel ratio). – Subroutine NEWOF is called for each fuel-air mixture read from an AFINP namelist. Calculations are done if this is the beginning of a case or if air-fuel ratio AF is different from the value used in the previous cycle.

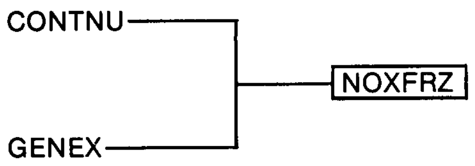
Some of the calculations are the same as those done in a routine by the same name in the CEC program (ref. 1). These combine the fuel and air into a set of properties for the total reactant. Some data are printed out.

NEWOF also calculates the properties and composition of the initial charge. Initial estimates for the level 1 combustion calculations are also set.



NOXFRZ (NO_x freeze). – NOXFRZ is an entry in AJCOEF which is used to freeze and unfreeze the species NO. Nitric oxide is frozen after combustion for level 1 and 2 cycles. No NO freezing is done for levels 3 to 5.

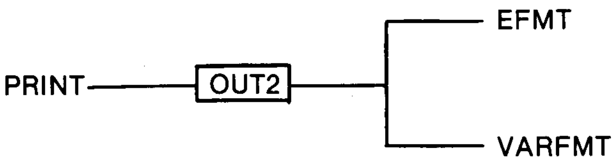
Freezing is accomplished by treating NO as a component. The current number of components NLM is adjusted. When NO is frozen, NLM = L1; otherwise, NLM = L1 – 1.



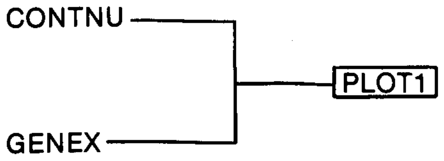
OOUT (Otto output). – Subroutine OOUT has two entries, HEAD and PRINT. OOUT has no executable statements apart from those associated with its entries.

OUT1 (output 1). – OUT1 writes information for the fuels and air in a format similar to the reactant cards in the input. It also prints the fuel-air mixtures. This information appears on the summary sheets for all levels.

OUT2 (output 2). – OUT2 is an entry to a routine in OUT1 which prints many of the mixture properties appearing in the columns printed on the level 1 summary sheets and the intermediate output for the higher levels. The routine is similar to the routine of the same name in reference 1.



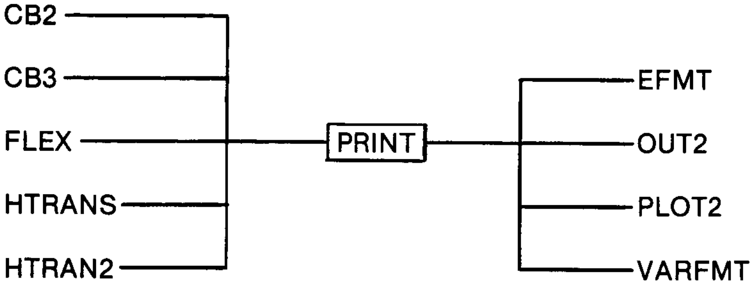
PLOT1 (plotting 1). – PLOT1 is an entry to a routine in PLT which is called at the beginning of each nonideal cycle to initialize some indices for use with PLOT2, which sets variables for plotting.



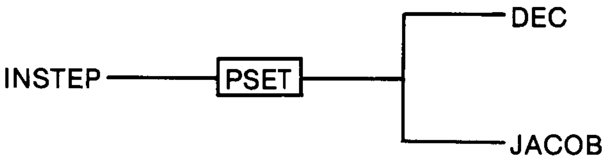
PLOT2 (plotting 2). – PLOT2 is an entry to a routine in PLT. It sets the variables saved for plotting at the intermediate output points during the nonideal cycles. These variables are tabulated and defined in table VII and stored in the COMMON labeled PLTS.

PLT (plotting). – PLT initializes some plotting variables at the beginning of an initial run.

PRINT (printing). – PRINT is an entry to a routine in OOUT. For nonideal cycles it calls PLOT2 for storing some mixture properties and compositions at intermediate output points. These data are printed for all levels when the intermediate output option is being used. Data are always printed for the converged ideal cycle.



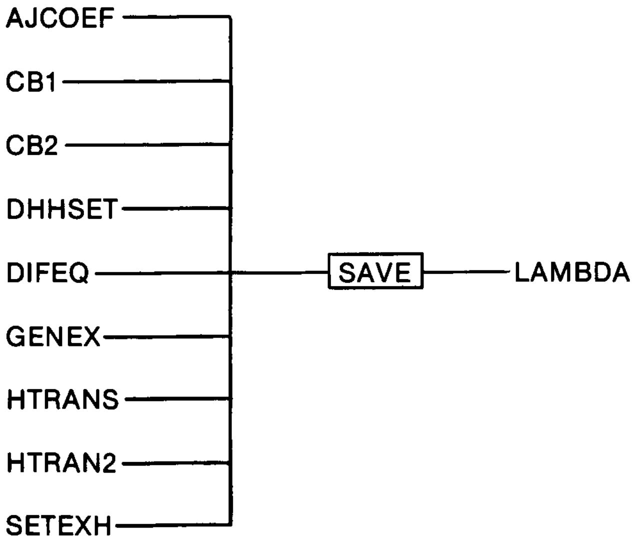
PSET. – Routine PSET evaluates the matrix used in the solution of the integration equations. Apart from a couple of minor name changes this routine is identical to Hindmarsh's PSET (ref. 4).



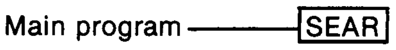
REACT (reactants). – REACT reads and processes the data on the reactant cards in the case input. The routine is similar to the routine of the same name in reference 1.

RSTART (restart). – RSTART reads the labeled COMMON data from I/O unit 7 one cycle at a time until the point is reached where the calculations are to continue.

SAVE (save data). – Part of subroutine SAVE is similar to the routine of the same name in the Gordon-McBride program CEC (ref. 1). This is the part that saves compositions or uses compositions from a previous point for initial estimates for the current point NPT. It has been modified to use thermodynamic derivatives to correct the compositions from the previous point for current conditions. These corrections are given by equations (III-29) and (III-30).

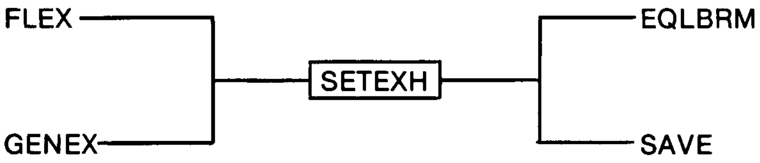


SEAR (search). – Subroutine SEAR is very similar to subroutine SEARCH in reference 1. It searches the thermodynamic data on I/O unit 4 for appropriate product species for the current chemical system and stores the data in common. The data are described in appendix A.



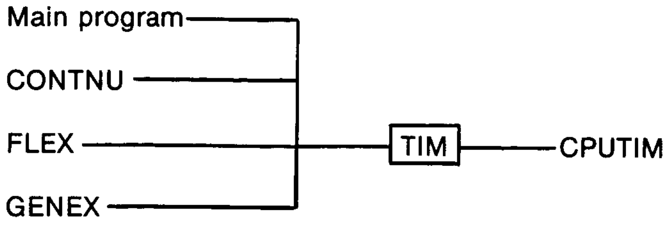
SETEXH (set exhaust). – SETEXH is an entry in subroutine AJCOEF. The routine saves exhaust gas compositions and several exhaust gas properties for output and later use. By using the mole fractions the thermodynamic coefficients of the individual species are combined into a single set to represent the composite exhaust gas.

An equilibrium calculation is done by using an assigned temperature of 298.15 K and an assigned pressure equal to the exhaust pressure PEXH. The resulting enthalpy HEQL is used in calculating exhaust power, equation (III-106), and exhaust efficiency, equation (III-105), which appear on the summary sheets in the output.

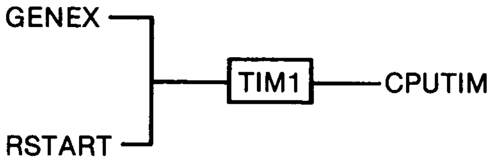


SOL (solve). – This routine is identical to Hindmarsh's routine SOL (ref. 4), which, in turn, is virtually identical to Moler's routine SOLVE (ref. 5). It backsolves a system of linear equations which have been reduced to upper triangular form by DEC.

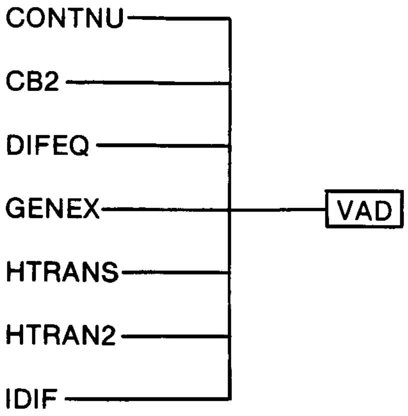
TIM (time). – TIM is used to calculate the time between the current call and a previous call to the routine. It requires a user-supplied routine CPUTIM. See the writeup for CPUTIM.



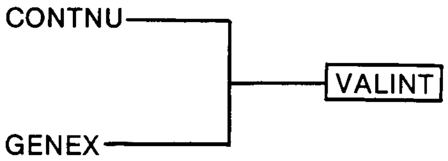
TIM1 (time 1). – TIM1 is called once prior to calculations for levels greater than 1. It sets an initial value in calculating cycle times. It requires a user-supplied routine CPUTIM. See the writeup for CPUTIM.



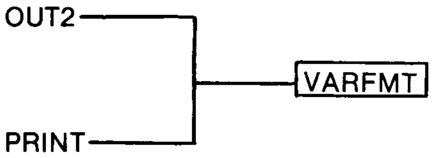
VAD (volume, area, and derivatives). – VAD calculates cylinder area and volume and their derivatives with respect to crankangle by using equations (I-86), (I-88), and (III-21).



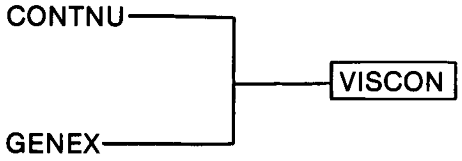
VALINT (valve initialization). – VALINT is an entry in subroutine FLOW. The routine initializes poppet valve flow parameters and reads the FLOWIN namelist in the case input.



VARFMT (variable format). – VARFMT is the same as the subroutine by the same name in the Gordon-McBride program CEC (ref. 1). It adjusts the number of decimal places in the format according to the size of the number for many of the tabulated output numbers.



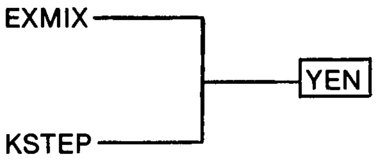
VISCON (viscosity and conductivity). – VISCON is an entry in subroutine HTCS. It reads the transport data coefficients as detailed in appendix B from I/O unit 8 and stores the appropriate data for up to 30 species. The data are also added to the case output on unit 6. The KCV array is used to index the species in the kinetic data order of species, and the ICV array is used for the thermodynamic order. See HTCS for additional information. The transport properties coefficients are set to zero for species without any transport data. Molecular weights are also calculated for species with nonzero transport properties.



VONLY (viscosity only). – VONLY is an entry in HTCS to share that part of HTCS which calculates shear viscosities only. See HTCS writeup for a more complete description.

YCHG (Y change). – YCHG is an entry in subroutine CLRY. For levels 4 and 5 it is called at the end of combustion to remove the differential equation for the unburned-gas temperature and to add equations for the number of moles of fuel and air. Subroutine KSTEP sets INDEX equal to –2 and calls INTEX, where JSTART is set to –2. JSTART = –2 then triggers INSTEP to call YCHG.

YEN (move compositions from Y array to EN array). – Subroutine YEN copies the integration results into storages used by the rest of the program.



BLOCK DATA. – BLOCK DATA is very similar to the one used in the Gordon-McBride program CEC (ref. 1). The universal gas constant (ref. 31) was updated and moved to BLOCK DATA. Also the atomic weights (ref. 32) were updated.

TABLE I. - INPUT/OUTPUT DATA FILES

Logical unit	Data file	Input/ output	Modeling levels	Detailed description
4	Thermodynamic properties	Input	1-5	Appendix A
5	Case input	Input	1-5	Section "Case input" and tables II to VI
6	Case output	Output	1-5	Section "Case output"
7	Plot and restart	(a)	2-5	Section "Plot and restart dump"
8	Transport properties	Input	[b]4-5	Appendix B
9	Chemical kinetics	Input	3-5	Appendix C

[a] This data file is output for an initial run, input and output for a restart run, and input for a plotting program.

[b] Modeling levels 2 and 3 with a non-Eichelberg heat transfer coefficient ($c_2 \neq 0$ in eq. (I-105)) also require this file.

TABLE II. - SUMMARY OF CASE INPUT

Cards in order	Format	Optional	Comments
Initial run			
REAC code	A4	No	REAC in card columns 1 to 4. Indicates reactants to follow.
Reactant(s)	See table III	No	All reactants excluding air as described in table III.
Blank card		No	Indicates end of reactants.
OMIT card(s)	A4,11X,4(3A4,3X)	Yes	OMIT in card columns 1 to 4 and species names starting in columns 16, 31, 46, and 61 indicate that species in the thermodynamic data with these names will then be excluded from the calculations.
NAME code	A4	No	NAME in card columns 1 to 4. Indicates namelists to follow.
OTTINP namelist	----------	No	See table IV for list and description of variables.
AFINP namelist	----------	No	See table V for list and description of variables.
AFINP or FLOWIN namelists	----------	Yes	See note below for cases requiring this additional input and table VI for variables in FLOWIN namelist.
Restart run			
RESTART i	A4,A3,8A1	No	RESTART in columns 1 to 7. The integer *i* within the next eight columns indicates the cycle from which to restart calculations. If the integer field is blank, calculations continue from the last cycle calculated.
AFINP namelist	----------	No	See table V for list and description of variables.
AFINP or FLOWIN namelists	----------	Yes	(a)

[a] The following cases require additional namelists as indicated:

(1) Cycle-to-cycle variations in AFINP variables—An AFINP namelist will be read at the beginning of each nonideal cycle until VARAF = FALSE in AFINP.

(2) Cases using poppet valve flow equations (levels 4 and 5)—one of the variables IFLOW or KFLAME in the AFINP namelist is set to the first cycle where flow equations are to be used. FLOWIN must immediately follow the first AFINP, where IFLOW or KFLAME is set. See table VI for a description of the FLOWIN varaibles. Poppet flow cannot be turned off except by restart at some previous nonflow cycle.

TABLE III. - REACTANT CARDS

Contents (one card for each reactant fuel, maximum 14)	Format	Card columns
Atomic symbols and formula numbers (maximum, five sets)	5(A2,F7.5)	1-45
Relative weight of fuel in total fuels or number of moles	F7.5	46-52
Blank if previous item is relative weight or *M* if previous item is number of moles	A1	53
[a]Enthalpy, cal/mol (required for non-gaseous species)	F9.5	54-62
State: S, L, or G for solid, liquid, or gas, respectively	A1	63
Temperature, K	F7.0	64-70
Code to distinguish among species with the same formula, matches columns 17 and 18 on first thermodynamic data card for the species	A2	79-80

[a]See ref. 1 for a discussion of enthalpy base.

TABLE IV. – INPUT VARIABLES IN OTTINP NAMELIST

Program variable	Dimension	Type	Default	Optional ?	Mathematical symbol	Definition and comment
AN	8	R	0.	Yes	$a_n, n = 1,8$	Coefficients for Fourier burning law, eq. (I-92)
B1	1	R	1.	Yes	b_1	Parameter used in calculation of velocity for Re, eq. (I-108)
B2	1	R	0.	Yes	b_2	Parameter used in calculation of velocity for Re, eq. (I-108)
BETA	1	R	0.	Yes	β	Parameter required for Wiebe burning function, eqs. (I-99) to (I-101). Nonzero value triggers use of the Wiebe function. Parameter α is calculated from eq. (I-100).
BORE	1	R	1.	No	B	Cylinder bore, cm
CA	1	R	0.	(a)	$A(0)$	Combustion chamber surface area, cm^2, eq. (I-88)
CR	1	R	0.	No	r	Compression ratio
CSBURN	1	L	.FALSE.	Yes	-----	Cosine burn model[b]. Equivalent to AN(1) = 0.5 and AN(2) = −0.5
FREQ	1	R	0.	No	-----	Engine speed in revolutions per minute
HA	1	R	0.	Yes	a	Heat transfer coefficient parameter, eq. (I-105)
HB	1	R	0.	Yes	b	Heat transfer coefficient parameter, eq. (I-105)
HC1	1	R	0.	Yes	c_1	Heat transfer coefficient parameter, eq. (I-105)
HC2	1	R	0.	Yes	c_2	Heat transfer coefficient parameter, eq. (I-105)
HC3	1	R	0.	Yes	c_3	Heat transfer coefficient parameter, eq. (I-105)
HC4	1	R	0.	Yes	c_4	If HC1 = HC2 = HC3 = HC4 = 0, then HC4 is set to 1.250427×10^{-5} for Eichelberg heat transfer coefficient
HLEN	1	R	BORE value	Yes	D	Length parameter in Re, eq. (I-107)
HP	1	L	.FALSE.	Yes	-----	Pressure discontinuities calculated as a minimum internal energy change. See eq. (I-118)[b]
KASE	1	I	0	Yes	-----	Arbitrary case identification number
PEXH	1	R	0.	No	p_e	Exhaust pressure, atm
PFUEL	1	R	PEXH	Yes	p_F	Fuel pressure, atm
PMFOLD	1	R	0.	No	p_m	Manifold pressure, atm
RHUMID	1	R	0.	Yes	-----	Relative humidity. Values ≤ 1 assumed to be fractions, values > 1 assumed to be percentages of saturation humidity
ROD	1	R	0.	No	l	Connecting rod length, cm
SP	1	L	.TRUE.	Yes	-----	Pressure discontinuities calculated as an isentropic change, eq. (I-118)[b]
STROKE	1	R	0.	No	L	Piston stroke, cm
TAIR	1	R	298.15	Yes	-----	Air temperature, K
TRACE	1	R	0.	Yes	-----	Option to print mole fractions ≥ TRACE in special E-format
TW	1	R	0.	Yes[a]	T_w	Effective wall temperature, K

[a] Required for heat transfer calculations.

[b] If variable is set to true.

TABLE V. - INPUT VARIABLES IN AFINP NAMELIST

Program variable	Dimension	Type	Default	Optional ?	Mathematical symbol	Definition and comment
AF	1	R	-1.	Yes[a]	A/F	Air-fuel weight ratio
DEBUG	1	L	.FALSE.	Yes	-----	If variable is set to TRUE, print properties and compositions for (1) All ideal cycles (2) Crankangles throughout nonideal cycles
EGR	1	R	0.	Yes	E_G	Mass fraction of fresh charge from exhaust gas recirculation. Numbers >1 are divided by 100
EQRAT	1	R	-1.	Yes[a]	-----	Equivalence ratio based on oxidation states (eq. (204) in ref. 1)
FA	1	R	-1.	Yes[a]	F/A	Fuel-air weight ratio
FPCT	1	R	-1.	Yes[a]	-----	Percentage of fuel by weight
IFLOW	1	I	0	Yes	-----	First cycle for which poppet valve flow calculations begin (levels 4 and 5)
IPRINT	12	I	0	Yes	-----	List of cycle numbers for intermediate output (same as DEBUG = .TRUE. for those cycles)
KFLAME	1	I	9999	Yes	-----	First cycle for which a kinetic flame is used during combustion (level 5)
KINET	1	I	0	Yes	-----	First cycle with chemical kinetics during combustion and expansion (level 3)
NCYCLE	1	I	0	Yes	-----	Total number of nonideal cycles
NEWAVG	1	L	.FALSE.	Yes	-----	If variable is set to TRUE, cycle-averaged exhaust gas properties are reinitialized.
PHI	1	R	-1.	Yes[a]	-----	Equivalence ratio Φ: $(F/A)/(F/A)_{\text{stoichiometric}}$
SPARK	1	R	0.	Yes	θ_0	Ignition point in degrees before TDC
TAU	1	R	0.	Yes	τ	Relaxation time, sec, used with finite-burning-rate models, eq. (I-89). TAU>0 is required for Wiebe burning model, eqs. (I-99) to (I-101)
TEGR	1	R	[b]0.	Yes	-----	Temperature, K, of exhaust gas for EGR
THBURN	1	R	20.	Yes[c]	$\theta_f-\theta_0$	See symbol list, Chapter I
VARAF	1	L	.FALSE.	No	-----	Read another AFINP namelist before executing the next cycle if variable is set to TRUE

[a] At least one value of AF, EQRAT, FA, FPCT, or PHI must be given at the beginning of the problem. Value will remain constant unless changed in succeeding AFINP namelists.

[b] TEGR is initialized to zero but will be set to exhaust temperature of the previous cycle if no value is given and EGR$\neq$0.

[c] At least one value of THBURN must be given for the first nonideal cycle. The value may be zero for motoring or changed with succeeding AFINP namelists.

TABLE VI. - INPUT VARIABLES IN FLOWIN NAMELIST

Program variable[a]	Type	Default	Optional	Mathematical symbol	Definition[a] and comment
AIN(n), n = 1,3	R	1.,0,0	Yes	$A_n^{(+)}$, $n=1,3$	Parameters for normal intake flow
AINR(n), n = 1,3	R	1.,0,0	Yes	$A_n^{(+)}$, $n=1,3$	Parameters for reverse intake flow
AEX(n), n = 1,3	R	1.,0,0	Yes	$A_n^{(-)}$, $n=1,3$	Parameters for normal exhaust flow
AEXR(n), n = 1,3	R	1.,0,0	Yes	$A_n^{(-)}$, $n=1,3$	Parameters for reverse exhaust flow
BIN(n), n = 1,3	R	0,0,0	Yes	$b_n^{(+)}$, $n=1,3$	Parameters for normal intake flow
BINR(n), n = 1,3	R	0,0,0	Yes	$b_n^{(+)}$, $n=1,3$	Parameters for reverse intake flow
BEX(n), n = 1,3	R	0,0,0	Yes	$b_n^{(-)}$, $n=1,3$	Parameters for normal exhaust flow
BEXR(n), n = 1,3	R	0,0,0	Yes	$b_n^{(-)}$, $n=1,3$	Parameters for reverse exhaust flow
ALFAIN	R	Calculated	Yes	$\alpha^{(+)}$	Parameter in Reynolds number
ALFAEX	R	Calculated	Yes	$\alpha^{(-)}$	Parameter in Reynolds number
BETAIN	R	45.	No	$\beta^{(+)}$	Intake valve seat angle, deg
BETAEX	R	45.	No	$\beta^{(-)}$	Exhaust valve seat angle, deg
DIN	R	0.	No	$d^{(+)}$	Minimum intake valve diameter, cm
DEX	R	0.	No	$d^{(-)}$	Minimum exhaust valve diameter, cm
EIN(n), n = 1,4	R	0,0,0,0	Yes	$E_n^{(+)}$, $n=1,4$	Parameters for normal intake flow
EINR(n), n = 1,4	R	0,0,0,0	Yes	$E_n^{(+)}$, $n=1,4$	Parameters for reverse intake flow
EEX(n), n = 1,4	R	0,0,0,0	Yes	$E_n^{(-)}$, $n=1,4$	Parameters for normal exhaust flow
EEXR(n), n = 1,4	R	0,0,0,0	Yes	$E_n^{(-)}$, $n=1,4$	Parameters for reverse exhaust flow
IVOPEN	R	0.	No	$\theta_o^{(+)}$	Crankangle intake valve opens
IVSHUT	R	180.	No	$\theta_c^{(+)}$	Crankangle intake valve shuts
EVOPEN	R	540.	No	$\theta_o^{(-)}$	Crankangle exhaust valve opens
EVSHUT	R	720.	No	$\theta_c^{(-)}$	Crankangle exhaust valve shuts
LIN	R	$1.\times 10^{35}$	Yes	$l_0^{(+)}$	Parameter for normal intake flow
LINR	R	$1.\times 10^{35}$	Yes	$l_0^{(+)}$	Parameter for reverse intake flow
LEX	R	$1.\times 10^{35}$	Yes	$l_0^{(-)}$	Parameter for normal exhaust flow
LEXR	R	$1.\times 10^{35}$	Yes	$l_0^{(-)}$	Parameter for reverse exhaust flow
RIN(n), n = 1,10	R	0.	No	$r_n^{(+)}$, $n=1,10$	Parameter for intake flow
REX(n), n = 1,10	R	0.	No	$r_n^{(-)}$, $n=1,10$	Parameter for exhaust flow

[a] All variables are poppet valve flow parameters, eqs. (I-110) to (I-117).

TABLE VII. – VARIABLES STORED IN COMMON PLTS FOR PLOTTING

Program symbol	Dimension	Definition
PRESS	400	Pressure, atm
VOLUME	400	Volume, cm^3
CRANK	400	Crankangle, deg
TEMPB	400	Burned-gas temperature, K
TEMPUB	400	Unburned-gas temperature, K
CCO	400	CO concentration, mole percent (burned gas during combustion)
CNO	400	NO concentration, ppm by mole (burned gas during combustion)
QLM	400	Heat loss, J
DQDTH	400	Rate of heat loss, (J/K) × 100
WORKI	400	Indicated work, J
DWIDTH	400	Rate of indicated work, (J/K) × 100
WORKP	400	Pump work, J
DWPDTH	400	Rate of pump work, (J/K) × 100
MBURN	400	Mass fraction of burned gas
VBURN	400	Volume fraction of burned gas
MASS	400	Cylinder mass, g
XM3PI	1	Maximum mass during cycle, g
IND1	1	Number of values stored for each of the variables dimensioned (400 except TEMPB, TEMPUB, MBURN, and VBURN)
IND3	1	Number of TEMPB values. First TEMPB value is for angle CRANK (IND1 – IND3 + 1)
IND4	1	Number of TEMPUB values
IND7	1	Number of MBURN and VBURN values
ICYCNO	1	Cycle number
BURN	1	Logical variable which is only false for motoring cycle (i.e., THBURN = 0)
KASENO	1	Same as KASE in OTTINP namelist

TABLE VIII. – COMPARISON OF FIRST FOUR CUMULANTS AND k-STATISTICS FROM A PEARSON TYPE III DISTRIBUTION FOR SAMPLE SIZES N = 5000 AND N = 25

i	κ_i	$k_i(N=5000)$	$k_i(N=25)$
1	15.6787	15.6771	15.1074
2	4.1667	4.2067	2.9929
3	6.9445	7.2907	2.9432
4	17.3611	17.7222	–.3190

TABLE IX. - STEADY STATE RESULTS FROM CASE 222 AT A STOICHIOMETRIC AIR-FUEL RATIO

[Cycle-averaged properties for the six stoichiometric cycles 7 to 12 of case 222; net exhaust flow rate, 11.9576 g/sec; molecular weight, 28.4043; enthalpy, −1787.35 J/g.]

Constituent	Mass-averaged composition, mole fraction
Ar	0.008633
CO	.001291
CO_2	.114872
H	.000013
H_2	.000483
H_2O	.153976
NO	.000034
N_2	.719796
OH	.000052
O_2	.000848

TABLE X. - NONSTEADY RESULTS FROM CASE 222 FOR CYCLE-TO-CYCLE VARIATION IN AIR-FUEL RATIO

[Cycle-averaged properties for the 25 cycles 13 to 37 of case 222; net exhaust flow rate, 12.0165 g/sec; molecular weight, 28.0453; enthalpy, −1741.27 J/g.]

Constituent	Mass-averaged composition, mole fraction
Ar	0.008499
CO	.017712
CO_2	.101544
H	0
H_2	.007361
H_2O	.151719
NO	.000022
N_2	.708618
OH	.000021
O_2	.004115
CH_4	.000059
C_2H_2	.000314
C_2H_4	.000009

TABLE XI. – PROGRAM ROUTINES

Levels ≥ 1 (ideal and general)	Levels ≥ 2 (heat transfer and burning)	Levels ≥ 3 (chemical kinetics)	Levels ≥ 4 (poppet-valve flow)
Executive Main program GENEX CONTNU (GENEX) Input and initialization ADDAIR (AJCOEF) AIRSET (AJCOEF) GENEX REACT SEAR TIM1 (TIM) Equilibrium and frozen CPHS EQLBRM FROZEN GAUSS HCALC LAMBDA MATRIX SAVE Output EFMT HEAD (OOUT) OUT1 OUT2 (OUT1) VARFMT Miscellaneous AJCOEF CHARGE (AJCOEF) DHHSET (AJCOEF) EGRH (AJCOEF) MOVE (VAD) NOXFRZ (AJCOEF) SETEXH (AJCOEF) TIM CTIM (TIM)	Executive BRNEX HTRANS[a] HTRAN2 (HTRANS)[a] Input and initialization RSTART VISCON Burning BRNEX CB1 CB2 (CB1) CB3 (CB1) COMBIN (AJCOEF) FRBURN Transport properties and heat transfer coefficient HTCS VISCON (HTCS) Output DUMPCM PLOT1 (PLT) PLOT2 (PLT) PLT PRINT (OOUT) Miscellaneous DELTH (VAD)[a] VAD	Executive INTEX KSTEP Input and initialization IDIF (DIFEQ) KDATA Integration COSET DEC DIFEQ INSTEP INTEX JACOB PSET SOL Miscellaneous KWORK (DIFEQ) YCHG (CLRY) YEN	Executive FLEX Input and initialization VALINT (FLOW) Flow DMDTH EXMIX FLOW VONLY (HTCS) Miscellaneous CLRY FDTH

[a] Routine used for levels 2 and 3 only.

TABLE XII. - ASSIGNED STATES FOR SUBROUTINES EQLBRM AND FROZEN

Assigned states	Program variables	Definitions
Temperature and pressure	TT, PP, TP = .TRUE., VOL = .FALSE., HP = .FALSE., SP = .FALSE.	TT ≡ temperature, K; PP ≡ pressure, atm
Temperature and volume	TT, VLM (NPT), TP = .TRUE., VOL = .TRUE., HP = .FALSE., SP = .FALSE.	VLM (NPT) ≡ specific volume, cm^3/g mixture, for printed column NPT
Enthalpy and pressure	HSUB0, PP, HP = .TRUE., VOL = .FALSE., TP = .FALSE., SP = .FALSE.	HSUB0 ≡ assigned enthalpy/R, g-mole K/g mixture
Internal energy and volume	HSUB0, VLM (NPT), HP = .TRUE., VOL = .TRUE., TP = .FALSE., SP = .FALSE.	HSUB0 ≡ assigned internal energy/R, g-mole K/g mixture
Entropy and pressure	S0 for EQLBRM or SSUM (NPT) for FROZEN, PP, SP = .TRUE., VOL = .FALSE., TP = .FALSE., HP = .FALSE.	S0 or SSUM (NPT) ≡ assigned entropy/R, g-mole/g mixture, for column NPT
Entropy and volume	S0 for EQLBRM or SSUM (NPT) for FROZEN, VLM (NPT), SP = .TRUE., VOL = .TRUE., TP = .FALSE., HP = .FALSE.	Same as above

Appendix A
Thermodynamic Data

The thermodynamic data are given in the empirical form of equation (III-111). The data were obtained via the PAC2 computer program (ref. 6). The format and order of the data are given in table XIII. Sample sets used with the examples in appendixes D to I are given in tables XIV and XV.

TABLE XIII. – FORMAT FOR THERMODYNAMIC DATA ON LOGICAL UNIT 4

Card order	Contents	Format	Card columns
First card	Temperature ranges for two sets of coefficients: lowest T, common T, and highest T	3A4 3F10.3	1-6 1-30
Set of four cards for each product[a]	Species name	3A4	1-12
	Name code[b] (distinguishes among species with same name)	A2	17-18
	Date[b]	2A3	19-24
	Atomic symbols and numbers	4(A2,F3.0)	25-44
	Phase of species (S, L, or G for solid, liquid or gas, respectively)	A1	45
	Temperature range	2F10.3	46-65
	The integer 1[b]	I15	80
	Coefficients a_i ($i = 1$ to 5) for upper temperature interval	5(E15.8)	1-75
	The integer 2[b]	I5	80
	Coefficients a_6 and a_7 for upper temperature interval and a_1, a_2, and a_3 for lower temperature interval	5(E15.8)	1-75
	The integer 3[b]	I5	80
	Coefficients a_4, a_5, a_6, and a_7 for lower temperature interval	4(E15.8)	1-60
	The integer 4[b]	I20	80
Follows products	END	A3	1-3
Set for four cards for each fuel[c]	Same format as products		
Last card	END2	A4	1-4

[a] Gaseous species and condensed species with only one condensed phase can be in any order. However, the sets for two or more condensed phases of the same species must be adjacent. If there are more than two condensed phases of a species, their sets must be either in increasing or decreasing order according to their temperature intervals.

[b] Optional.

[c] Data for gaseous fuel must follow data for any liquid phase.

TABLE XIV. - THERMODYNAMIC DATA USED WITH EXAMPLES III, IV, AND VI

```
                                 Date file                                        | Reference
   300.000  1000.000  5000.000
AR                  L 5/66AR 1.00 0.00 0.00 0.G   300.000  5000.000                      7
 0.25000000E 01 0.00000000     0.00000000     0.00000000     0.00000000
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.00000000     0.00000000
 0.00000000     0.00000000    -0.74537498E 03 0.43660006E 01
C(S)                J 3/78C   1    0    0    0S   300.000  5000.000              1       7
   .14324054+01    .17555871-02   -.71889423-06    .14015109-09   -.10069094-13  2
  -.68498756+03   -.83936690+01   -.39942085+00    .50285536-02    .33566391-06  3
  -.47166280-08    .23510115-11   -.99185350+02    .14885486+01                  4
C                   J 3/61C   100  000  000  0G   300.000  5000.000              1       7
 0.25810663E 01-0.14696202E-03 0.74388084E-07-0.79481079E-11 0.58900977E-16      2
 0.85216294E 05 0.43128879E 01 0.25328705E 01-0.15887641E-03 0.30682082E-06      3
-0.26770064E-09 0.87488827E-13 0.85240422E 05 0.46062374E 01                     4
CH                  J12/67C   1H   10   00   0G   300.000  5000.000              1       7
 0.22673116E 01 0.22043000E-02-0.62250191E-06 0.69689940E-10-0.21274952E-14      2
 0.70838037E 05 0.87889352E 01 0.35632752E 01-0.20031372E-03-0.40129814E-06      3
 0.18226922E-08-0.86768311E-12 0.70405506E 05 0.17628023E 01                     4
CH2                 J12/72C   1H   2    0    0G   300.000  5000.000              1       7
 0.27525479E+01 0.39782047E-02-0.14921731E-05 0.25956899E-09-0.17110673E-13      2
 0.45547759E+05 0.66534799E+01 0.35883347E+01 0.21724137E-02-0.13323408E-05      3
 0.19469445E-08-0.89431394E-12 0.45315188E+05 0.22627869E+01                     4
CH20                J 3/61C   1H   20   10   0G   300.000  5000.000              1       7
 0.28364249E 01 0.68605298E-02-0.26882647E-05 0.47971258E-09-0.32118406E-13      2
-0.15236031E 05 0.78531169E 01 0.37963783E 01-0.25701785E-02 0.18548815E-04      3
-0.17869177E-07 0.55504451E-11-0.15088947E 05 0.47548163E 01                     4
CH20H               L 7/80C   1H   30   1    0G   300.000  5000.000              1      8,9
 0.46113930E 01 0.63004829E-02-0.20052776E-05 0.27953462E-09-0.13790255E-13      2
-0.38903362E 04 0.53708118E 00 0.32669954E 01 0.70455037E-02 0.19389763E-05      3
-0.48157496E-08 0.17366325E-11-0.33094617E 04 0.83675241E 01                     4
CH3                 J 6/69C   1H   30   00   0G   300.000  5000.000              1       7
 0.28400327E 01 0.60869086E-02-0.21740338E-05 0.36042576E-09-0.22725300E-13      2
 0.16449813E 05 0.55056751E 01 0.34666350E 01 0.38301845E-02 0.10116802E-05      3
-0.18859236E-08 0.66803182E-12 0.16313104E 05 0.24172192E 01                     4
CH30                L 6/80C   1H   30   1    0G   300.000  5000.000              1       8
 0.37590771E 01 0.78945048E-02-0.26710486E-05 0.39814507E-09-0.21447125E-13      2
 0.13208081E 03 0.29936295E 01 0.21097078E 01 0.71927756E-02 0.53939157E-05      3
-0.74311082E-08 0.20939578E-11 0.97822803E 03 0.13137219E 02                     4
CH30H               L 4/80C   1H   40   1    0G   300.000  5000.000              1      10
 0.40334730E 01 0.93680508E-02-0.30449373E-05 0.43456994E-09-0.22136329E-13      2
-0.26159859E 05 0.23539820E 01 0.26587849E 01 0.73515214E-02 0.71443337E-05      3
-0.87661114E-08 0.23805116E-11-0.25353684E 05 0.11238121E 02                     4
CH4                 J 3/61C   1H   400  000  0G   300.000  5000.000              1       7
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13      2
-0.99787078E 04 0.10707143E 02 0.38261932E 01-0.39794581E-02 0.24558340E-04      3
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00                     4
CN                  J 6/69C   1N   10   00   0G   300.000  5000.000              1       7
 0.36036285E 01 0.33644390E-03 0.10028933E-06-0.16318166E-10-0.36286722E-15      2
 0.51159833E 05 0.35454505E 01 0.37386307E 01-0.19239224E-02 0.47035189E-05      3
-0.31113000E-08 0.61675318E-12 0.51270927E 05 0.34490218E 01                     4
CO                  J 9/65C   10   100  000  0G   300.000  5000.000              1       7
 0.29840696E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14      2
-0.14245228E 05 0.63479156E 01 0.37100928E 01-0.16190964E-02 0.36923594E-05      3
-0.20319674E-08 0.23953344E-12-0.14356310E 05 0.29555351E 01                     4
C02                 J 9/65C   10   200  000  0G   300.000  5000.000              1       7
 0.44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13      2
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05      3
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01                     4
C2H                 J 3/67C   2H   100  000  0G   300.000  5000.000              1       7
 0.44207650E 01 0.22119303E-02-0.59294945E-06 0.94195775E-10-0.68527594E-14      2
 0.55835444E 05-0.11588093E 01 0.26499400E 01 0.84919515E-02-0.98165375E-05      3
 0.65373629E-08-0.17356273E-11 0.56275751E 05 0.76898609E 01                     4
C2H2                J 3/61C   2H   200  000  0G   300.000  5000.000              1       7
 0.45751083E 01 0.51238358E-02-0.17452354E-05 0.28673065E-09-0.17951426E-13      2
 0.25607428E 05-0.35737940E 01 0.14102768E 01 0.19057275E-01-0.24501390E-04      3
 0.16390872E-07-0.41345447E-11 0.26188208E 05 0.11393827E 02                     4
C2H3                CR2178C   2H   30   00   0G   300.000  50000.000             1      11
 3.91828714E+00 7.10447061E-03-1.98355545E-06 2.02007740E-10-3.95303041E-15      2
 3.22388006E+04 3.03714667E+00 3.65517039E+00 9.50926265E-03-9.48490849E-06      3
 1.03811014E-08-4.82336893E-12 3.22190821E+04 4.01239803E+00                     4
C2H4                L 4/80C   2H   4    0    0G   300.000  5000.000              1      12
 0.43843679E 01 0.96509494E-02-0.31845530E-05 0.46213655E-09-0.24069342E-13      2
 0.41205039E 04-0.23853559E 01 0.11654673E 01 0.13374992E-01 0.25754771E-05      3
-0.10187399E-07 0.43603341E-11 0.53428867E 04 0.15699718E 02                     4
C2H5                L 8/78C   2H   5    0    0G   300.000  5000.000              1      13
   .66807245+00    .18731209-01   -.79184728-05    .15267665-08   -.10733175-12  2
   .12119230+05    .21040679+02    .66807245+00    .18731209-01   -.79184728-05  3
   .15267665-08   -.10733175-12    .12119230+05    .21040679+02                  4
C2H6                L 2/80C   2H   6'   0    0G   300.000  5000.000              1      14,9
 0.47258701E 01 0.14017530E-01-0.46358909E-05 0.67257888E-09-0.34934695E-13      2
-0.12780930E 05-0.46865377E 01 0.14893150E 01 0.15296880E-01 0.62937688E-05      3
-0.13133693E-07 0.47989243E-11-0.11342469E 05 0.14320247E 02                     4
C3H7                CR2178C   3H   70   00   0G   300.000  5000.000              1      11
 2.63075453E+00 2.42979573E-02-9.62786424E-06 1.71216523E-09-1.12767794E-13      2
 9.17147226E+03 1.08721288E+01 3.43473677E+00 1.89905564E-02 2.26298908E-06      3
-9.34591044E-09 3.55787331E-12 9.08796344E+03 7.48875556E+00 0.                  4
```

TABLE XIV. - Concluded.

```
                                  Date file                                           Reference

C3H8              L 4/80C   3H    8     0     0G    300.000  5000.000          1    14,9
 0.75252171E 01 0.18890340E-01-0.62839244E-05 0.91793728E-09-0.48124099E-13    2
-0.16464547E 05-0.17843903E 02 0.89692080E 00 0.26689861E-01 0.54314251E-05    3
-0.21260007E-07 0.92433301E-11-0.13954918E 05 0.19355331E 02                   4
H                 J 3/77H   1     0     0     0G    300.000  5000.000          1    7
   .25000000+01   .00000000      .00000000      .00000000      .00000000       2
   .25474390+05  -.45989841+00   .25000000+01   .00000000      .00000000       3
   .00000000      .00000000      .25474390+05  -.45989841+00                   4
HCN               L12/69H   1C    1N    10    0G    300.000  5000.000          1    15
 0.37068121E 01 0.33382803E-02-0.11913320E-05 0.19992917E-09-0.12826452E-13    2
 0.14962636E 05 0.20794904E 01 0.24513556E 01 0.87208371E-02-0.10094203E-04    3
 0.67255698E-08-0.17626959E-11 0.15213002E 05 0.80830085E 01                   4
HCO               J12/70H   1C    10    10    0G    300.000  5000.000          1    7
 0.34738348E+01 0.34370227E-02-0.13632664E-05 0.24928645E-09-0.17044331E-13    2
 0.39594005E+04 0.60453340E+01 0.38840192E+01-0.82974448E-03 0.77900809E-05    3
-0.70616962E-08 0.19971730E-11 0.40563860E+04 0.48354133E+01                   4
HO2               J 9/78H   10    2     0     0G    300.000  5000.000          1    7
   .40173060+01   .22175883-02  -.57710171-06   .71372882-10  -.36458591-14    2
  -.11412445+04   .37846051+01   .35964102+01   .52500748-03   .75118344-05    3
  -.95674952-08   .36597628-11  -.89333502+03   .66372671+01                   4
H2                J 3/77H   2     0     0     0G    300.000  5000.000          1    7
   .30558123+01   .59740400-03  -.16747471-08  -.21247544-10   .25195487-14    2
  -.86168476+03  -.17207073+01   .29432327+01   .34815509-02  -.77713819-05    3
   .74997496-08  -.25203379-11  -.97695413+03  -.18186137+01                   4
H2O(L)            J 3/79H   20    1     0     0L    273.150   500.000          1    7
   .00000000      .00000000      .00000000      .00000000      .00000000       2
   .00000000      .00000000      .28630800+02  -.20260986+00   .78529479-03    3
  -.13653020-05   .91326966-09  -.38579539+05  -.11895046+03                   4
H2O               J 3/79H   20    1     0     0G    300.000  5000.000          1    7
   .26340654+01   .31121899-02  -.90278449-06   .12673054-09  -.69164732-14    2
  -.29876258+05   .70823873+01   .41675564+01  -.18106868-02   .59450878-05    3
  -.48670871-08   .15284144-11  -.30289546+05  -.73087997+00                   4
H2O2              L 6/80H   20    2     0     0G    300.000  5000.000          1    16,9
 0.48067904E 01 0.36028353E-02-0.10963122E-05 0.14431741E-09-0.65176204E-14    2
-0.18137465E 05-0.58927882E 00 0.34637089E 01 0.54991394E-02 0.10543617E-05    3
-0.47568385E-08 0.21907606E-11-0.17673590E 05 0.68011646E 01                   4
N                 J 3/77N   1     0     0     0G    300.000  5000.000          1    7
   .24370811+01   .13233886-03  -.90907754-07   .22864054-10  -.13762291-14    2
   .56128585+05   .45211111+01   .25000004+01  -.31078154-08   .83216097-11    3
  -.94278278-14   .38108039-17   .56106975+05   .41806431+01                   4
NCO               J12/70N   1C    10    10    0G    300.000  5000.000          1    7
 0.49964357E+01 0.26250880E-02-0.10928387E-05 0.20309111E-09-0.13915195E-13    2
 0.17379356E+05-0.17325320E+01 0.31092021E+01 0.66201022E-02-0.26070086E-05    3
-0.14560380E-08 0.10922032E-11 0.17977514E+05 0.83561334E+01                   4
NH                J 6/77N   1H    1     0     0G    300.000  5000.000          1    7
   .27414945+01   .14032028-02  -.46001046-06   .80217694-10  -.52770870-14    2
   .44499551+05   .59638059+01   .34520634+01   .54983583-03  -.20358506-05    3
   .30336916-08  -.12401129-11   .44249545+05   .20208741+01                   4
NH2               J 6/77N   1H    2     0     0G    300.000  5000.000          1    7
   .27554321+01   .32905847-02  -.11160410-05   .20903758-09  -.15676329-13    2
   .22001133+05   .69276497+01   .41262894+01  -.16485841-02   .56461668-05    3
  -.40505222-08   .10499871-11   .21697548+05   .16960494+00                   4
NH3               J 6/77N   1H    3     0     0G    300.000  5000.000          1    7
   .23168577+01   .62841460-02  -.21251163-05   .34018690-09  -.21470026-13    2
  -.64265487+04   .82987657+01   .37729747+01  -.82975716-03   .11801882-04    3
  -.12126874-07   .41763790-11  -.66908514+04   .14968947+01                   4
NO                J 6/63N   10    100   000   0G    300.000  5000.000          1    7
 0.31890000E 01 0.13382281E-02-0.52899318E-06 0.95919332E-10-0.64847932E-14    2
 0.98283290E 04 0.67458126E 01 0.40459521E 01-0.34181783E-02 0.79819190E-05    3
-0.61139316E-08 0.15919076E-11 0.97453934E 04 0.29974988E 01                   4
NO2               J 9/64N   10    200   000   0G    300.000  5000.000          1    7
 0.46240771E 01 0.25260332E-02-0.10609498E-05 0.19879239E-09-0.13799384E-13    2
 0.22899900E 04 0.13324138E 01 0.34589236E 01 0.20647064E-02 0.66866067E-05    3
-0.95556725E-08 0.36195881E-11 0.28152265E 04 0.83116983E 01                   4
N2                J 3/77N   2     0     0     0G    300.000  5000.000          1    7
   .28532899+01   .16022128-02  -.62936893-06   .11441022-09  -.78057465-14    2
  -.89008093+03   .63964897+01   .37044177+01  -.14218753-02   .28670392-05    3
  -.12028885-08  -.13954677-13  -.10640795+04   .22336285+01                   4
O                 J 3/77O   1     0     0     0G    300.000  5000.000          1    7
   .25342961+01  -.12478170-04  -.12562724-07   .69029862-11  -.63797095-15    2
   .29231108+05   .49628591+01   .30309401+01  -.22525853-02   .39824540-05    3
  -.32604921-08   .10152035-11   .29136526+05   .26099342+01                   4
OH                J 6/77O   1H    1     0     0G    300.000  5000.000          1    7
   .28897814+01   .10005879-02  -.22048807-06   .20191288-10  -.39409831-15    2
   .38857042+04   .55566427+01   .38737300+01  -.13393772-02   .16348351-05    3
  -.52133639-09   .41826974-13   .35802348+04   .34202406+00                   4
O2                J 3/77O   2     0     0     0G    300.000  5000.000          1    7
   .36122139+01   .74853166-03  -.19820647-06   .33749008-10  -.23907374-14    2
  -.11978151+04   .36703307+01   .37837135+01  -.30233634-02   .99492751-05    3
  -.98189101-08   .33031825-11  -.10638107+04   .36416345+01                   4
END
C3H8              L 4/80C   3H    8     0     0G    300.000  5000.000          1    14,9
 0.75252171E 01 0.18890340E-01-0.62839244E-05 0.91793728E-09-0.48124099E-13    2
-0.16464547E 05-0.17843903E 02 0.89692080E 00 0.26689861E-01 0.54314251E-05    3
-0.21260007E-07 0.92433301E-11-0.13954918E 05 0.19355331E 02                   4
END2
```

TABLE XV. - THERMODYNAMIC DATA USED WITH EXAMPLES I, II, AND V

```
                               Date file                                         Reference
   300.000  1000.000  5000.000
AR                 L 5/66AR 1.00 0.00 0.00 0.G   300.000  5000.000                    7
 0.25000000E 01 0.00000000      0.00000000     0.00000000     0.0000000
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.00000000     0.0000000
 0.00000000     0.00000000    -0.74537498E 03 0.43660006E 01
C(S)               J 3/78C   1    0    0    0S   300.000  5000.000             1      7
   .14324054+01    .17555871-02  -.71889423-06   .14015109-09  -.10069094-13   2
  -.68498756+03  -.83936690+01  -.39942085+00   .50285536-02   .33566391-06   3
  -.47166280-08    .23510115-11  -.99185350+02   .14885486+01                  4
CH4                J 3/61C  1.H  4.00 0.00 0.G   300.000  5000.000                    7
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13
-0.99787078E 04 0.10707143E 02 0.38261932E 01-0.39794581E-02 0.24558340E-04
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00
CO                 J 9/65C  1.0  1.00 0.00 0.G   300.000  5000.000                    7
 0.29840696E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14
-0.14245228E 05 0.63479156E 01 0.37100928E 01-0.16190964E-02 0.36923594E-05
-0.20319674E-08 0.23953344E-12-0.14356310E 05 0.29555351E 01
CO2                J 9/65C  1.0  2.00 0.00 0.G   300.000  5000.000                    7
 0.44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01
H                  J 3/77H   1    0    0    0G   300.000  5000.000             1      7
   .25000000+01    .00000000      .00000000      .00000000      .00000000      2
   .25474390+05  -.45989841+00    .25000000+01   .00000000      .00000000      3
   .00000000      .00000000      .25474390+05  -.45989841+00                  4
HO2                J 9/78H  10    2    0    0G   300.000  5000.000             1      7
   .40173060+01    .22175883-02  -.57710171-06   .71372882-10  -.36458591-14   2
  -.11412445+04    .37846051+01   .35964102+01   .52500748-03   .75118344-05   3
  -.95674952-08    .36597628-11  -.89333502&03   .66372671&01                  4
H2                 J 3/77H   2    0    0    0G   300.000  5000.000             1      7
   .30558123+01    .59740400-03  -.16747471-08  -.21247544-10   .25195487-14   2
  -.86168476+03  -.17207073+01   .29432327+01   .34815509-02  -.77713819-05   3
   .74997496-08  -.25203379-11  -.97695413+03  -.18186137+01                  4
H2O(L)             J 3/79H  20    1    0    0L   273.150   500.000             1      7
   .00000000      .00000000      .00000000      .00000000      .00000000      2
   .00000000      .00000000      .28630800+02  -.20260986+00   .78529479-03   3
  -.13653020-05    .91326966-09  -.38579539+05  -.11895046+03                  4
H2O                J 3/79H  20    1    0    0G   300.000  5000.000             1      7
   .26340654+01    .31121899-02  -.90278449-06   .12673054-09  -.69164732-14   2
  -.29876258+05    .70823873+01   .41675564+01  -.18106868-02   .59450878-05   3
  -.48670871-08    .15284144-11  -.30289546+05  -.73087997+00                  4
NH3                J 6/77N  1H    3    0    0G   300.000  5000.000             1      7
   .23168577+01    .62841460-02  -.21251163-05   .34018690-09  -.21470026-13   2
  -.64265487+04    .82987657+01   .37729747+01  -.82975716-03   .11801882-04   3
  -.12126874-07    .41763790-11  -.66908514+04   .14968947+01                  4
N                  J 3/77N   1    0    0    0G   300.000  5000.000             1      7
   .24370811+01    .13233886-03  -.90907754-07   .22864054-10  -.13762291-14   2
   .56128585+05    .45211111+01   .25000004+01  -.31078154-08   .83216097-11   3
  -.94278278-14    .38108039-17   .56106975+05   .41806431+01                  4
NO                 J 6/63N  1.0  1.00 0.00 0.G   300.000  5000.000                    7
 0.31890000E 01 0.13382281E-02-0.52899318E-06 0.95919332E-10-0.64847932E-14
 0.98283290E 04 0.67458126E 01 0.40459521E 01-0.34181783E-02 0.79819190E-05
-0.61139316E-08 0.15919076E-11 0.97453934E 04 0.29974988E 01
NO2                J 9/64N  1.0  2.00 0.00 0.G   300.000  5000.000                    7
 0.46240771E 01 0.25260332E-02-0.10609498E-05 0.19879239E-09-0.13799384E-13
 0.22899900E 04 0.13324138E 01 0.34589236E 01 0.20647064E-02 0.66866067E-05
-0.95556725E-08 0.36195881E-11 0.28152265E 04 0.83116983E 01
N2                 J 3/77N   2    0    0    0G   300.000  5000.000             1      7
   .28532899+01    .16022128-02  -.62936893-06   .11441022-09  -.78057465-14   2
  -.89008093+03    .63964897+01   .37044177+01  -.14218753-02   .28670392-05   3
  -.12028885-08  -.13954677-13  -.10640795+04   .22336285+01                  4
O                  J 3/77O   1    0    0    0G   300.000  5000.000             1      7
   .25342961+01  -.12478170-04  -.12562724-07   .69029862-11  -.63797095-15   2
   .29231108+05    .49628591+01   .30309401+01  -.22525853-02   .39824540-05   3
  -.32604921-08    .10152035-11   .29136526+05   .26099342+01                  4
OH                 J 6/77O  1H    1    0    0G   300.000  5000.000             1      7
   .28897814+01    .10005879-02  -.22048807-06   .20191288-10  -.39409831-15   2
   .38857042+04    .55566427+01   .38737300+01  -.13393772-02   .16348351-05   3
  -.52133639-09    .41826974-13   .35802348+04   .34202406+00                  4
O2                 J 3/77O   2    0    0    0G   300.000  5000.000             1      7
   .36122139+01    .74853166-03  -.19820647-06   .33749008-10  -.23907374-14   2
  -.11978151+04    .36703307+01   .37837135+01  -.30233634-02   .99492751-05   3
  -.98189101-03    .33031825-11  -.10638107+04   .36416345+01                  4
END                          0.   0.   0.   0.      0.000     0.000
CH3OH              L 4/80C  1H   4O    1    0G   300.000  5000.000             1     10
 0.40334730E 01 0.93680508E-02-0.30449373E-05 0.43456994E-09-0.22136329E-13   2
-0.26159859E 05 0.23539820E 01 0.26587849E 01 0.73515214E-02 0.71443337E-05   3
-0.87661114E-08 0.23805116E-11-0.25353684E 05 0.11238121E 02                  4
C2H5OH             L12/73C  2H   6O    1    0G   300.000  1000.000             1     17
 0.             0.             0.             0.             0.               2
 0.             0.             0.20453260E+01 0.18097289E-01 0.11356807E-04   3
-0.25318665E-07 0.10843493E-10-0.29665177E+05 0.16637635E+02                  4
```

TABLE XV. - Concluded.

```
                                  Date file                                               Reference

C3H8              L 4/80C    3H    8     0     0G    300.000  5000.000               1     14,9
 0.75252171E 01 0.18890340E-01-0.62839244E-05 0.91793728E-09-0.48124099E-13          2
-0.16464547E 05-0.17843903E 02 0.89692080E 00 0.26689861E-01 0.54314251E-05          3
-0.21260007E-07 0.92433301E-11-0.13954918E 05 0.19355331E 02                         4
C3H7OH            L12/73C    3H    80    1     0G    300.000  1000.000               1     17
 0.             0.             0.             0.             0.                      2
 0.             0.             0.28935102E+01 0.22546234E-01 0.18912669E-04          3
-0.35990505E-07 0.14751417E-10-0.32800045E+05 0.15191566E+02                         4
C6H6(L)           A10/80C    6H    6     0     0L    280.000   360.000               1     18
    .00000000      .00000000       .00000000       .00000000       .00000000         2
    .00000000      .00000000       .59257575+01    .64273539-01   -.16683048-03      3
    .23024018-06   .00000000       .22923560+04   -.26683081+02                      4
C6H6              A10/80C    6H    6     0     0G    300.000  1500.000               1     18
   -.38339763+02   .17191041+00   -.18189276-03    .91061601-07   -.17497493-10      2
    .17191013+05   .21160786+03   -.46950488+01    .58501890-01   -.33443458-04      3
   -.17341596-09   .50520230-11    .90663077+04    .43156568+02                      4
C7H8(L)           A10/80C    7H    8     0     0L    250.000   380.000               1     18
    .00000000      .00000000       .00000000       .00000000       .00000000         2
    .00000000      .00000000       .21823676+02   -.80604340-01    .32872833-03      3
   -.30544066-06   .00000000      -.37821298+04   -.85638471+02                      4
C7H8              A10/80C    7H    8     0     0G    300.000  1500.000               1     18
   -.70146091+02   .28641896+00   -.31440621-03    .16070293-06   -.31273750-10      2
    .20509824+05   .37449350+03   -.34057115+01    .60445642-01   -.20292121-04      3
   -.16381350-07   .10929382-10    .45485187+04    .40860881+02                      4
C8H16             L 9/74C    8H    16    0     0G    300.000  1500.000               1     19
-0.19137314E 02 0.69371462E-01 0.67576038E-04-0.10115679E-06 0.31757513E-10          2
-0.29994805E 04 0.15213559E 03 0.27015257E 01 0.63744605E-01 0.10288634E-04          3
-0.51851664E-07 0.23527721E-10-0.13609438E 05 0.21171082E 02                         4
C8H18(L)          A10/80C    8H    18    0     0L    220.000   300.000               1     18
    .00000000      .00000000       .00000000       .00000000       .00000000         2
    .00000000      .00000000       .71413393+02   -.50207950+00    .18341990-02      3
   -.20450165-05   .00000000      -.41243725+05   -.27722240+03                      4
C8H18             A10/80C    8H    18    0     0G    300.000  1000.000               1     18
    .00000000      .00000000       .00000000       .00000000       .00000000         2
    .00000000      .00000000       .28209642+01    .62381281-01    .34503217-04      3
   -.83254430-07   .35431926-10   -.28886853+05    .20621261+02                      4
H2                J 3/61H    20    00    00    0G    300.000  5000.000               1      7
 0.31001901E 01 0.51119464E-03 0.52644210E-07-0.34909973E-10 0.36945345E-14          2
-0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.58099162E-05          3
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01                         4
AR                L 5/66AR 1.00 0.00 0.00 0.G    300.000  5000.000                      7
 0.25000000E 01 0.00000000     0.00000000     0.00000000     0.00000000
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.00000000     0.00000000
 0.00000000     0.00000000    -0.74537498E 03 0.43660006E 01
CO2               J 9/65C  1.0  2.00 0.00 0.G    300.000  5000.000                      7
 0 44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01
N2                J 3/77N    2     0     0     0G    300.000  5000.000               1      7
    .28532899+01   .16022128-02   -.62936893-06    .11441022-09   -.78057465-14      2
   -.89008093+03   .63964897+01    .37044177+01   -.14218753-02    .28670392-05      3
   -.12028885-08  -.13954677-13   -.10640795+04    .22336285+01                      4
O2                J 3/77O    2     0     0     0G    300.000  5000.000               1      7
    .36122139+01   .74853166-03   -.19820647-06    .33749008-10   -.23907374-14      2
   -.11978151+04   .36703307+01    .37837135+01   -.30233634-02    .99492751-05      3
   -.98164101-08   .33031825-11   -.10638107+04    .36416345+01                      4
NH3               J 6/77N    1H    3     0     0G    300.000  5000.000               1      7
    .23168577+01   .62841460-02   -.21251163-05    .34018690-09   -.21470026-13      2
   -.64265487+04   .82987657+01    .37729747+01   -.82975716-03    .11801882-04      3
   -.12126874-07   .41763790-11   -.66908514+04    .14968947+01                      4
END2
```

Appendix B

Transport Data

Shear viscosities and thermal conductivities for some of the pure species which appear in the six sample calculations were obtained from a number of sources. The compilation of Svehla (ref. 20) was used for the species CH_4, C_2H_2, C_2H_4, C_3H_8, and C_6H_6. The computer program TRAN76 by Svehla and McBride (ref. 21) was the source of the transport properties for NO, O, H, NO_2, OH, and CO. The values for N_2 and O_2 were taken from Hanley and Ely (ref. 22). The values for H_2O and NH_3 were taken from Sanford Gordon (ref. 33). Shear viscosities for H_2, Ar, and CO_2 were obtained from a paper by Maitland and Smith (ref. 23). Conductivities for H_2 were obtained from the computer program TRAN76; for Ar we selected the values of Svehla (ref. 20) and for CO_2 we faired a curve through experimental data assembled by Svehla from more than 20 papers. These data were fit by least squares to an equation of the form (III-113). The equations for N_2, O_2, CO_2, and Ar were used to calculate transport properties for air (Chapter III, in the section Fresh Charge Specification) by the mixing rules (I-152) to (I-155). The results of this calculation were also represented in a least squares sense. The data representations for the complete set of species and air are shown in table XVI.

The format for the data is given in table XVII. The cards may be in any order, with the last card having LAST in card columns 1 to 4.

TABLE XVI. - TRANSPORT DATA FOR GASEOUS SPECIES USED WITH THE EXAMPLES

AIR	0.632169E 00	-0.218525E 02	-0.324679E 04	0.172670E 01	VISC
AIR	0.642016E 00	-0.222573E 03	0.307023E 05	0.861183E 00	COND
H2	0.687200E 00	-0.617320E 00	-0.111490E 03	0.577240E 00	VISC
H2	0.116129E 01	0.469043E 03	-0.551496E 05	-0.149041E 01	COND
CH3OH	0.641455E 00	-0.211775E 03	0.125265E 05	0.150983E 01	VISC
CH3OH	0.793792E 00	-0.487550E 03	0.322097E 05	0.646522E 00	COND
CH4	0.600440E 00	-0.817476E 02	0.165196E 04	0.154710E 01	VISC
CH4	0.853201E 00	-0.288931E 03	0.193692E 05	0.355349E 00	COND
C2H2	0.579032E 00	-0.152664E 03	0.628889E 04	0.177748E 01	VISC
C2H2	0.666734E 00	-0.330498E 03	0.165066E 05	0.118596E 01	COND
C2H4	0.578808E 00	-0.148526E 03	0.598107E 04	0.175623E 01	VISC
C2H4	0.674458E 00	-0.506382E 03	0.309615E 05	0.150224E 01	COND
C3H8	0.578645E 00	-0.156438E 03	0.658750E 04	0.156557E 01	VISC
C3H8	0.638223E 00	-0.615207E 03	0.349529E 05	0.183162E 01	COND
C6H6	0.611472E 00	-0.214866E 03	0.120814E 05	0.144145E 01	VISC
C6H6	0.549565E 00	-0.765765E 03	0.437054E 05	0.222155E 01	COND
NO	0.646504E 00	0.388567E 01	-0.858737E 04	0.165204E 01	VISC
NO	0.614175E 00	-0.260319E 03	0.360173E 05	0.110633E 01	COND
N2	0.633933E 00	-0.119153E 02	-0.471490E 04	0.166605E 01	VISC
N2	0.686393E 00	-0.161885E 03	0.236277E 05	0.482688E 00	COND
AR	0.590770E 00	-0.925770E 02	0.299040E 04	0.233077E 01	VISC
AR	0.641113E 00	-0.670283E 01	-0.730294E 04	0.207105E 00	COND
O	0.763927E 00	0.569723E 02	-0.345462E 04	0.822320E 00	VISC
O	0.776744E 00	0.803466E 02	-0.349619E 04	-0.481407E-01	COND
H	0.860209E 00	0.498177E 02	-0.542523E 04	-0.102874E 01	VISC
H	0.869708E 00	0.670316E 02	-0.828927E 04	0.891354E 00	COND
H2O	0.756380E 00	-0.301892E 03	0.187539E 05	0.987951E 00	VISC
H2O	0.123241E 01	-0.163667E 03	0.141541E 05	-0.291285E 01	COND
NH3	0.596434E 00	-0.314839E 03	0.271390E 05	0.197019E 01	VISC
NH3	0.774738E 00	-0.627003E 03	0.664059E 05	0.974813E 00	COND
NO2	0.603384E 00	-0.988315E 02	-0.969625E 03	0.200464E 01	VISC
NO2	0.504502E 00	-0.475725E 03	0.415525E 05	0.201241E 01	COND
OH	0.597497E 00	-0.365001E 03	0.351359E 05	0.217217E 01	VISC
OH	0.812287E 00	-0.264930E 03	0.343595E 05	0.105187E 00	COND
CO	0.779825E 00	0.193974E 03	-0.317845E 05	0.436375E 00	VISC
CO	0.800546E 00	-0.237400E 02	0.804541E 04	-0.468414E 00	COND
CO2	0.440370E 00	-0.288400E 03	0.193120E 05	0.324659E 01	VISC
CO2	0.603518E 00	-0.438483E 03	0.322949E 05	0.134023E 01	COND
O2	0.659260E 00	0.941422E 00	-0.711780E 04	0.164432E 01	VISC
O2	0.478050E 00	-0.452958E 03	0.579015E 05	0.228192E 01	COND
LAST					

TABLE XVII. – FORMAT FOR TRANSPORT DATA OF GASEOUS SPECIES ON LOGICAL UNIT 8

Card columns	Format	Contents
1	1X	Not used
2 to 13	3A4	Name used with thermodynamic data
14 to 28	E15.4	a_1 in eq. (III-113)
29 to 43	E15.4	a_2 in eq. (III-113)
44 to 58	E15.4	a_3 in eq. (III-113)
59 to 73	E15.4	a_4 in eq. (III-113)
74 to 76	3X	Not used
77 to 80	A4	VISC for shear viscosity or COND for thermal conductivity

Appendix C

Chemical Kinetic Data

We have assembled two reaction mechanisms with the sole intention of using them to illustrate modeling at levels 3 to 5. These mechanisms have simply been culled from the literature, and we make no claim to critical evaluation. The first mechanism is a short, 19-reaction mechanism for burned-gas chemistry for use at levels 3 and 4 of examples I and II. It is shown as table XVIII in this appendix. Reactions (1) and (3) to (9) are from the critically evaluated compilations of Baulch et al. (refs. 24 and 25). Reactions (10) to (14) are taken from the critically evaluated compilation of Hampson and Garvin (ref. 26). The remaining reactions come from a mechanism used by Bittker and Wolfbrandt (ref. 27).

The second mechanism is a longer, 121-reaction mechanism for the combustion of propane and is used for level 5 of examples IV and VI. It is shown as table XIX of this appendix. The first 84 reactions form the methanol oxidation mechanism of Westbrook and Dryer (ref. 28), which includes their methane and ethane mechanisms. Reactions (85) to (88) and (90) to (105) were chosen from a propane mechanism given by Wakelyn, Jachimowski, and Wilson (ref. 29), reactions (106) to (110) come from Hampson and Garvin (ref. 26), reactions (113) to (121) are from a mechanism used by Duxbury and Pratt (ref. 30), and the remaining reactions were taken from Bittker and Wolfbrandt (ref. 27).

The input consists of two types of cards: reactions and third-body efficiencies. All reactions with the format given in table XX must precede the third-body efficiencies. A blank card signals the end of the reaction set. The format for the third-body efficiencies is given in table XXI and a blank card also signals the end of this set.

TABLE XVIII. - GAS PHASE CHEMICAL KINETICS MECHANISM USED WITH EXAMPLES I AND II

```
REACTION MECHANISM AND RATES (MOLES/CM**3 -SEC)
         K = A*T**N *EXP(-E/RT)
                                                                          A            N    E(CAL/MOLE)

  1) 1.0   CO      + 1.0   OH      =  1.0   CO2     + 1.0   H          0.6310E 08     1.3      -765.0
  2) 1.0   CO      + 1.0   O2      =  1.0   CO2     + 1.0   O          0.1200E 12     0.0     35000.0
  3) 1.0   H       + 1.0   O2      =  1.0   OH      + 1.0   O          0.2200E 15     0.0     16790.0
  4) 1.0   O       + 1.0   H2      =  1.0   OH      + 1.0   H          0.1800E 11     1.0      8900.0
  5) 1.0   H2      + 1.0   OH      =  1.0   H2O     + 1.0   H          0.2200E 14     0.0      5150.0
  6) 1.0   O       + 1.0   H2O     =  2.0   OH      + 0.0              0.6800E 14     0.0     18360.0
  7) 1.0   H       + 1.0   O2      =  1.0   HO2     + 0.0   M          0.1500E 16     0.0     -1000.0
  8) 0.0   M       + 1.0   O2      =  2.0   O       + 0.0              0.1800E 19    -1.0    118000.0
  9) 1.0   H       + 1.0   OH      =  1.0   H2O     + 0.0   M          0.8400E 22    -2.0         0.0
 10) 1.0   HO2     + 1.0   NO      =  1.0   NO2     + 1.0   OH         0.1200E 14     0.0      2380.0
 11) 1.0   O       + 1.0   NO2     =  1.0   NO      + 1.0   O2         0.1000E 14     0.0       596.0
 12) 1.0   NO      + 1.0   O       =  1.0   NO2     + 0.0   M          0.5620E 16     0.0     -1160.0
 13) 1.0   NO2     + 1.0   H       =  1.0   NO      + 1.0   OH         0.2900E 15     0.0       795.0
 14) 1.0   O       + 1.0   N2      =  1.0   NO      + 1.0   N          0.7800E 14     0.0     75500.0
 15) 1.0   N       + 1.0   O2      =  1.0   NO      + 1.0   O          0.6400E 10     1.0      6250.0
 16) 1.0   N       + 1.0   OH      =  1.0   NO      + 1.0   H          0.4000E 14     0.0         0.0
 17) 1.0   OH      + 1.0   HO2     =  1.0   H2O     + 1.0   O2         0.5000E 14     0.0      1000.0
 18) 1.0   O       + 1.0   HO2     =  1.0   OH      + 1.0   O2         0.5000E 14     0.0      1000.0
 19) 1.0   H       + 1.0   HO2     =  2.0   OH      + 0.0              0.2500E 15     0.0      1890.0

THIRD BODY EFFICIENCIES

     1.0   H       + 1.0   O2      =  1.0   HO2     + 0.0   M       O2        2.000  N2         2.000
     1.0   H       + 1.0   O2      =  1.0   HO2     + 0.0   M       H2O      32.500  CO2        7.500
     1.0   H       + 1.0   O2      =  1.0   HO2     + 0.0   M       CO        2.000             0.000
     1.0   H       + 1.0   OH      =  1.0   H2O     + 0.0   M       O2        1.600  H2O       20.000
     1.0   H       + 1.0   OH      =  1.0   H2O     + 0.0   M       CO        1.600  CO2        7.500
     1.0   H       + 1.0   OH      =  1.0   H2O     + 0.0   M       N2        1.600             0.000
```

TABLE XIX. - GAS-PHASE CHEMICAL KINETICS MECHANISM USED WITH EXAMPLES IV AND VI

REACTION MECHANISM AND RATES (MOLES/CM**3 -SEC)
K = A*T**N *EXP(-E/RT)

										A	N	E(CAL/MOLE)
1)	1.0	CH3OH	+ 0.0	M	=	1.0	CH3	+ 1.0	OH	0.3162E 19	0.0	80000.0
2)	1.0	CH3OH	+ 1.0	O2	=	1.0	CH2OH	+ 1.0	HO2	0.3981E 14	0.0	50900.0
3)	1.0	CH3OH	+ 1.0	OH	=	1.0	CH2OH	+ 1.0	H2O	0.3981E 13	0.0	2000.0
4)	1.0	CH3OH	+ 1.0	O	=	1.0	CH2OH	+ 1.0	OH	0.1585E 13	0.0	2300.0
5)	1.0	CH3OH	+ 1.0	H	=	1.0	CH2OH	+ 1.0	H2	0.3162E 14	0.0	7000.0
6)	1.0	CH3OH	+ 1.0	H	=	1.0	CH3	+ 1.0	H2O	0.5012E 13	0.0	5300.0
7)	1.0	CH3OH	+ 1.0	CH3	=	1.0	CH2OH	+ 1.0	CH4	0.1995E 12	0.0	9800.0
8)	1.0	CH3OH	+ 1.0	HO2	=	1.0	CH2OH	+ 1.0	H2O2	0.6309E 13	0.0	19400.0
9)	1.0	CH2OH	+ 0.0	M	=	1.0	CH2O	+ 1.0	H	0.2512E 14	0.0	29000.0
10)	1.0	CH2OH	+ 1.0	O2	=	1.0	CH2O	+ 1.0	HO2	0.1000E 13	0.0	6000.0
11)	1.0	CH4	+ 0.0	M	=	1.0	CH3	+ 1.0	H	0.1259E 18	0.0	88400.0
12)	1.0	CH4	+ 1.0	H	=	1.0	CH3	+ 1.0	H2	0.1259E 15	0.0	11900.0
13)	1.0	CH4	+ 1.0	OH	=	1.0	CH3	+ 1.0	H2O	0.3162E 04	3.1	2000.0
14)	1.0	CH4	+ 1.0	O	=	1.0	CH3	+ 1.0	OH	0.1585E 14	0.0	9200.0
15)	1.0	CH4	+ 1.0	HO2	=	1.0	CH3	+ 1.0	H2O2	0.1995E 14	0.0	18000.0
16)	1.0	CH3	+ 1.0	HO2	=	1.0	CH3O	+ 1.0	OH	0.1585E 14	0.0	0.0
17)	1.0	CH3	+ 1.0	OH	=	1.0	CH2O	+ 1.0	H2	0.3981E 13	0.0	0.0
18)	1.0	CH3	+ 1.0	O	=	1.0	CH2O	+ 1.0	H	0.1259E 15	0.0	2000.0
19)	1.0	CH3	+ 1.0	O2	=	1.0	CH3O	+ 1.0	O	0.2512E 14	0.0	29000.0
20)	1.0	CH2O	+ 1.0	CH3	=	1.0	CH4	+ 1.0	HCO	0.1000E 11	0.5	6000.0
21)	1.0	CH3	+ 1.0	HCO	=	1.0	CH4	+ 1.0	CO	0.3162E 12	0.5	0.0
22)	1.0	CH3	+ 1.0	HO2	=	1.0	CH4	+ 1.0	O2	0.1000E 13	0.0	400.0
23)	1.0	CH3O	+ 0.0	M	=	1.0	CH2O	+ 1.0	H	0.5012E 14	0.0	21000.0
24)	1.0	CH3O	+ 1.0	O2	=	1.0	CH2O	+ 1.0	HO2	0.1000E 13	0.0	6000.0
25)	1.0	CH2O	+ 0.0	M	=	1.0	HCO	+ 1.0	H	0.5012E 17	0.0	72000.0
26)	1.0	CH2O	+ 1.0	OH	=	1.0	HCO	+ 1.0	H2O	0.5012E 15	0.0	6300.0
27)	1.0	CH2O	+ 1.0	H	=	1.0	HCO	+ 1.0	H2	0.3981E 13	0.0	3800.0
28)	1.0	CH2O	+ 1.0	O	=	1.0	HCO	+ 1.0	OH	0.5012E 14	0.0	4600.0
29)	1.0	CH2O	+ 1.0	HO2	=	1.0	HCO	+ 1.0	H2O2	0.1000E 13	0.0	8000.0
30)	1.0	HCO	+ 1.0	OH	=	1.0	CO	+ 1.0	H2O	0.1000E 15	0.0	0.0
31)	1.0	HCO	+ 0.0	M	=	1.0	H	+ 1.0	CO	0.1585E 15	0.0	19000.0
32)	1.0	HCO	+ 1.0	H	=	1.0	CO	+ 1.0	H2	0.1995E 15	0.0	0.0
33)	1.0	HCO	+ 1.0	O	=	1.0	CO	+ 1.0	OH	0.1000E 15	0.0	0.0
34)	1.0	HCO	+ 1.0	HO2	=	1.0	CH2O	+ 1.0	O2	0.1000E 15	0.0	3000.0
35)	1.0	HCO	+ 1.0	O2	=	1.0	CO	+ 1.0	HO2	0.3162E 13	0.0	7000.0
36)	1.0	CO	+ 1.0	OH	=	1.0	CO2	+ 1.0	H	0.1259E 08	1.3	-800.0
37)	1.0	CO	+ 1.0	HO2	=	1.0	CO2	+ 1.0	OH	0.1000E 15	0.0	23000.0
38)	1.0	CO	+ 1.0	O	=	1.0	CO2	+ 0.0	M	0.6309E 16	0.0	4100.0
39)	1.0	CO2	+ 1.0	O	=	1.0	CO	+ 1.0	O2	0.2512E 13	0.0	43800.0
40)	1.0	H	+ 1.0	O2	=	1.0	O	+ 1.0	OH	0.1995E 15	0.0	16800.0
41)	1.0	H2	+ 1.0	O	=	1.0	H	+ 1.0	OH	0.1995E 11	1.0	8900.0
42)	1.0	H2O	+ 1.0	O	=	1.0	OH	+ 1.0	OH	0.3162E 14	0.0	18400.0
43)	1.0	H2O	+ 1.0	H	=	1.0	H2	+ 1.0	OH	0.1000E 15	0.0	20300.0
44)	1.0	H2O2	+ 1.0	OH	=	1.0	H2O	+ 1.0	HO2	0.1000E 14	0.0	1800.0
45)	1.0	H2O	+ 0.0	M	=	1.0	H	+ 1.0	OH	0.1995E 17	0.0	105100.0
46)	1.0	H	+ 1.0	O2	=	1.0	HO2	+ 0.0	M	0.1585E 16	0.0	-1000.0
47)	1.0	HO2	+ 1.0	O	=	1.0	OH	+ 1.0	O2	0.5012E 14	0.0	1000.0
48)	1.0	HO2	+ 1.0	H	=	2.0	OH	+ 0.0		0.2512E 15	0.0	1900.0
49)	1.0	HO2	+ 1.0	H	=	1.0	H2	+ 1.0	O2	0.2512E 14	0.0	700.0
50)	1.0	HO2	+ 1.0	OH	=	1.0	H2O	+ 1.0	O2	0.5012E 14	0.0	1000.0
51)	1.0	H2O2	+ 1.0	O2	=	2.0	HO2	+ 0.0		0.3981E 14	0.0	42600.0
52)	1.0	H2O2	+ 0.0	M	=	1.0	OH	+ 1.0	OH	0.1259E 18	0.0	45500.0
53)	1.0	H2O2	+ 1.0	H	=	1.0	HO2	+ 1.0	H2	0.1585E 13	0.0	3800.0
54)	1.0	O	+ 1.0	H	=	1.0	OH	+ 0.0	M	0.1000E 17	0.0	0.0
55)	1.0	O2	+ 0.0	M	=	2.0	O	+ 0.0		0.5012E 16	0.0	115000.0
56)	1.0	H2	+ 0.0	M	=	2.0	H	+ 0.0		0.1995E 15	0.0	96000.0
57)	1.0	C2H6	+ 0.0		=	2.0	CH3	+ 0.0		0.2512E 20	-1.0	88300.0
58)	1.0	C2H6	+ 1.0	CH3	=	1.0	C2H5	+ 1.0	CH4	0.5012E 00	4.0	8300.0
59)	1.0	C2H6	+ 1.0	H	=	1.0	C2H5	+ 1.0	H2	0.5012E 03	3.5	5200.0
60)	1.0	C2H6	+ 1.0	OH	=	1.0	C2H5	+ 1.0	H2O	0.6310E 14	0.0	2400.0
61)	1.0	C2H6	+ 1.0	O	=	1.0	C2H5	+ 1.0	OH	0.2512E 14	0.0	6400.0
62)	1.0	C2H5	+ 0.0		=	1.0	C2H4	+ 1.0	H	0.3981E 14	0.0	38000.0
63)	1.0	C2H5	+ 1.0	O2	=	1.0	C2H4	+ 1.0	HO2	0.1000E 13	0.0	5000.0
64)	1.0	C2H5	+ 1.0	C2H3	=	1.0	C2H4	+ 1.0	C2H4	0.3162E 18	0.0	35600.0
65)	1.0	C2H4	+ 1.0	O	=	1.0	CH3	+ 1.0	HCO	0.1000E 14	0.0	1100.0

TABLE XIX. - Concluded.

```
 66) 1.0  C2H4   + 0.0  M      =  1.0  C2H3  + 1.0  H          0.3981E 18    0.0   98200.0
 67) 1.0  C2H4   + 1.0  H      =  1.0  C2H3  + 1.0  H2         0.6310E 14    0.0    6000.0
 68) 1.0  C2H4   + 1.0  OH     =  1.0  C2H3  + 1.0  H2O        0.1000E 15    0.0    3500.0
 69) 1.0  C2H4   + 1.0  O      =  1.0  CH2O  + 1.0  CH2        0.2512E 14    0.0    5000.0
 70) 1.0  C2H3   + 0.0  M      =  1.0  C2H2  + 1.0  H          0.3162E 17    0.0   40500.0
 71) 1.0  C2H2   + 0.0  M      =  1.0  C2H   + 1.0  H          0.1000E 15    0.0  114000.0
 72) 1.0  C2H2   + 1.0  O2     =  2.0  HCO   + 0.0             0.3981E 13    0.0   28000.0
 73) 1.0  C2H2   + 1.0  H      =  1.0  C2H   + 1.0  H2         0.1995E 15    0.0   19000.0
 74) 1.0  C2H2   + 1.0  OH     =  1.0  C2H   + 1.0  H2O        0.6309E 13    0.0    7000.0
 75) 1.0  C2H2   + 1.0  O      =  1.0  C2H   + 1.0  OH         0.3162E 16   -0.6   17000.0
 76) 1.0  C2H2   + 1.0  O      =  1.0  CH2   + 1.0  CO         0.6310E 14    0.0    4000.0
 77) 1.0  C2H    + 1.0  O2     =  1.0  HCO   + 1.0  CO         0.1000E 14    0.0    7000.0
 78) 1.0  C2H    + 1.0  O      =  1.0  CO    + 1.0  CH         0.5012E 14    0.0       0.0
 79) 1.0  CH2    + 1.0  O2     =  1.0  HCO   + 1.0  OH         0.1000E 15    0.0    3700.0
 80) 1.0  CH2    + 1.0  O      =  1.0  CH    + 1.0  OH         0.1995E 12    0.7   25000.0
 81) 1.0  CH2    + 1.0  H      =  1.0  CH    + 1.0  H2         0.2512E 12    0.7   25700.0
 82) 1.0  CH2    + 1.0  OH     =  1.0  CH    + 1.0  H2O        0.2512E 12    0.7   25700.0
 83) 1.0  CH     + 1.0  O2     =  1.0  CO    + 1.0  OH         0.1259E 12    0.7   25700.0
 84) 1.0  CH     + 1.0  O2     =  1.0  HCO   + 1.0  O          0.1000E 14    0.0       0.0
 85) 0.0  M      + 1.0  C3H8   =  1.0  C2H5  + 1.0  CH3        0.5000E 16    0.0   65010.0
 86) 1.0  OH     + 1.0  C3H8   =  1.0  H2O   + 1.0  C3H7       0.1600E 15    0.0    3140.0
 87) 1.0  H      + 1.0  C3H8   =  1.0  H2    + 1.0  C3H7       0.6300E 14    0.0    8000.0
 88) 1.0  O      + 1.0  C3H8   =  1.0  OH    + 1.0  C3H7       0.5000E 14    0.0   10000.0
 89) 1.0  CH2    + 1.0  O2     =  1.0  CH2O  + 1.0  O          0.1000E 15    0.0    3700.0
 90) 1.0  CH3    + 1.0  C3H8   =  1.0  CH4   + 1.0  C3H7       0.2000E 14    0.0   10300.0
 91) 0.0         + 1.0  C3H7   =  1.0  C2H4  + 1.0  CH3        0.4000E 14    0.0   33100.0
 92) 1.0  O      + 1.0  CH3    =  1.0  OH    + 1.0  CH2        0.1900E 12    0.7   25700.0
 93) 1.0  H      + 1.0  CH3    =  1.0  H2    + 1.0  CH2        0.2700E 12    0.7   25700.0
 94) 1.0  OH     + 1.0  CH3    =  1.0  H2O   + 1.0  CH2        0.2700E 12    0.7   25700.0
 95) 1.0  CH     + 1.0  N2     =  1.0  HCN   + 1.0  N          0.1500E 12    0.0   19000.0
 96) 1.0  CN     + 1.0  H2     =  1.0  HCN   + 1.0  H          0.6000E 14    0.0    5300.0
 97) 1.0  O      + 1.0  HCN    =  1.0  OH    + 1.0  CN         0.1400E 12    0.7   16900.0
 98) 1.0  OH     + 1.0  HCN    =  1.0  CN    + 1.0  H2O        0.2000E 12    0.6    5000.0
 99) 1.0  CN     + 1.0  O2     =  1.0  NCO   + 1.0  O          0.3200E 14    0.0    1004.0
100) 1.0  CN     + 1.0  CO2    =  1.0  NCO   + 1.0  CO         0.3700E 13    0.0       0.0
101) 1.0  H      + 1.0  NCO    =  1.0  NH    + 1.0  CO         0.2000E 14    0.0       0.0
102) 1.0  NH     + 1.0  OH     =  1.0  N     + 1.0  H2O        0.5000E 12    0.5    1999.0
103) 1.0  O      + 1.0  NCO    =  1.0  NO    + 1.0  CO         0.2000E 14    0.0       0.0
104) 1.0  N      + 1.0  NCO    =  1.0  N2    + 1.0  CO         0.1000E 14    0.0       0.0
105) 1.0  CH     + 1.0  CO2    =  1.0  HCO   + 1.0  CO         0.3700E 13    0.0       0.0
106) 1.0  HO2    + 1.0  NO     =  1.0  NO2   + 1.0  OH         0.1200E 14    0.0    2380.0
107) 1.0  O      + 1.0  NO2    =  1.0  NO    + 1.0  O2         0.1000E 14    0.0     596.0
108) 1.0  NO     + 1.0  O      =  1.0  NO2   + 0.0  M          0.5620E 16    0.0   -1160.0
109) 1.0  NO2    + 1.0  H      =  1.0  NO    + 1.0  OH         0.2900E 15    0.0     795.0
110) 1.0  O      + 1.0  N2     =  1.0  NO    + 1.0  N          0.7800E 14    0.0   75500.0
111) 1.0  N      + 1.0  O2     =  1.0  NO    + 1.0  O          0.6400E 10    1.0    6250.0
112) 1.0  N      + 1.0  OH     =  1.0  NO    + 1.0  H          0.4000E 14    0.0       0.0
113) 1.0  NH3    + 1.0  OH     =  1.0  NH2   + 1.0  H2O        0.4000E 11    0.7    1100.0
114) 1.0  NH3    + 1.0  H      =  1.0  NH2   + 1.0  H2         0.5000E 12    0.5    1990.0
115) 1.0  NH3    + 1.0  O      =  1.0  NH2   + 1.0  OH         0.1500E 13    0.0    6000.0
116) 1.0  NH2    + 1.0  NO     =  1.0  N2    + 1.0  H2O        0.1000E 14    0.0       0.0
117) 1.0  NH2    + 1.0  OH     =  1.0  NH    + 1.0  H2O        0.3000E 11    0.7    1300.0
118) 1.0  NH2    + 1.0  H      =  1.0  NH    + 1.0  H2         0.1000E 12    0.7    4290.0
119) 1.0  NH2    + 1.0  O      =  1.0  NH    + 1.0  OH         0.9200E 12    0.5       0.0
120) 1.0  NH2    + 1.0  NH2    =  1.0  NH3   + 1.0  NH         0.2000E 12    0.6    3590.0
121) 1.0  NH     + 1.0  O2     =  1.0  NO    + 1.0  OH         0.1000E 11    0.0       0.0


THIRD BODY EFFICIENCIES

     1.0  H      + 1.0  O2     =  1.0  HO2   + 0.0  M      O2        2.000  N2      2.000
     1.0  H      + 1.0  O2     =  1.0  HO2   + 0.0  M      H2O      32.500  CO2     7.500
     1.0  H      + 1.0  O2     =  1.0  HO2   + 0.0  M      CO        2.000          0.000
     1.0  H2O    + 0.0  M      =  1.0  H     + 1.0  OH     O2        1.600  H2O    20.000
     1.0  H2O    + 0.0  M      =  1.0  H     + 1.0  OH     CO        1.600  CO2     7.500
     1.0  H2O    + 0.0  M      =  1.0  H     + 1.0  OH     N2        1.600          0.000
```

TABLE XX. - FORMAT FOR REACTION CARDS IN CHEMICAL KINETIC DATA

Card columns	Format	Contents
1-3	F3.1	Stoichiometric coefficient of reactant 1[a]
4-11	2A4	Name of reactant 1 or letter *M* for third-body decomposition reaction[b]
12	1X	Not read, but the symbol "+" may be used
13-15	F3.1	Stoichiometric coefficient of reactant 2[a]
16-23	2A4	Name of reactant 2 or letter *M* for third-body decomposition reaction[b]
24	1X	Not used
25	A1	Equal sign for reversible reaction or letter *R* for irreversible reaction
26-28	F3.1	Stoichiometric coefficient of product 1[a]
29-36	2A4	Name of product 1 or letter *M* for third-body recombination reaction[b]
37	1X	Not read, but symbol "+" may be used
38-40	F3.1	Stoichiometric coefficient of product 2[a]
41-48	2A4	Name of product 2 or letter *M* for third-body recombination reaction[b]
49	1X	Not used
50-60	E11.4	Factor *A* in rate equation $k=AT^N \exp(-E/RT)$
61-70	F10.4	*N* in above rate equation
71-80	F10.4	Activation energy *E* in above rate equation, cal/mole

[a] May be left blank (1) if stoichiometric coefficient is 1 or (2) if *M* is used in name position that follows.

[b] Names or letter *M* must be left adjusted. Names must match those used in the thermodynamic data. The letter *M* may be in either reactant or product name position.

TABLE XXI. - FORMAT FOR THIRD-BODY EFFICIENCY CARDS

Card columns	Format	Contents
1-48	(a)	Same as on corresponding reaction card
49-56	2A4	Name of third-body species
57	1X	Not read
58-63	F6.3	Efficiency value
64-65	2X	Not read
66-73	2A4	Name of third-body species
74	1X	Not read
75-80	F6.3	Efficiency value

[a] See Table XX.

Appendix D

Example I (Cases 512 and 513)

Input, Case 512

```
REAC
C 8.      H 18.                                         .42            L298.15  F
C 7.      H 8.                                          .38            L298.15  F
C 6.      H 6.                                          .18            L298.15  F
NAME
 &OTTINP FREQ=2140,BORE=10.16,STROKE=8.839,ROD=14.478,CA=80.,
 TW=360.,CR= 8.5,CSBURN=T,KASE=512,
 PEXH=.9840,PMFOLD=.5264,
   HC3=0.,HA=.0,HB=.0,HC2=.0000,
   SP=T,RHUMID=55.,TAIR=298.15&END
 &AFINP PHI=.725,SPARK=28.0,EGR=0.,THBURN=88.8,
   NCYCLE=8,KINET=4,TAU=0.00E-00,DEBUG=T,VARAF=F&END
```

Output, Case 512

Calculation Parameters

```
REAC
C    8.0000  H   18.0000      0.0000      0.0000      0.0000    0.420000       0.00  L    298.150     F
C    7.0000  H    8.0000      0.0000      0.0000      0.0000    0.380000       0.00  L    298.150     F
C    6.0000  H    6.0000      0.0000      0.0000      0.0000    0.180000       0.00  L    298.150     F
NAME

SPECIES BEING CONSIDERED (THERMODYNAMIC ORDER)
L 5/66  AR              J 3/78  C(S)         J 3/61  CH4         J 9/65  CO            J 9/65  CO2
J 3/77  H               J 9/78  HO2          J 3/77  H2          J 3/79  H2O(L)        J 3/79  H2O
J 6/77  NH3             J 3/77  N            J 6/63  NO          J 9/64  NO2           J 3/77  N2
J 3/77  O               J 6/77  OH           J 3/77  O2
&OTTINP
CR= 8.50
FREQ= 2140.0
CA= 80.0
BORE= 10.160
STROKE= 8.8390
ROD= 14.4780
TW= 360.0
HP= F
SP= T
TRACE= 0.0
TAIR= 298.1499
CSBURN= T
HC1= 0.0
HC2= 0.0
HC3= 0.0
HC4= 0.0
HA= 0.0
HB= 0.0
PFUEL= 0.0
PMFOLD= 0.52640
PEXH= 0.9840
KASE= 512
AN= 0.50, -0.50, 6*0.0
BETA= 0.0
IOUNIT= 5
HLEN= 0.0
B1= 1.0
B2= 0.0
RHUMID= 55.0
&END
&AFINP
VARAF= F
AF= -1.0
EQRAT= -1.0
PHI= 0.7250
FPCT= -1.0
FA= -1.0
THBURN= 88.79999
EGR= 0.0
SPARK= 28.0
TEGR= 0.0
TAU= 0.0
DEBUG= T
KINET= 4
IOUNIT= 5
NCYCLE= 8
IPRINT= 12*0
MODN= 0
KFLAME= 99999
IFLOW= 0
&END
```

```
FUELS

  C6H6(L)       A10/80
  C6H6          A10/80
  C7H8(L)       A10/80
  C7H8          A10/80
  C8H18(L)      A10/80
  C8H18         A10/80



REACTION MECHANISM AND RATES (MOLES/CM**3 -SEC)
         K = A*T**N *EXP(-E/RT)
                                                                                A            N   E(CAL/MOLE)

  1) 1.0   CO      + 1.0   OH       =  1.0   CO2     + 1.0   H             0.6310E 08      1.3     -765.0
  2) 1.0   CO      + 1.0   O2       =  1.0   CO2     + 1.0   O             0.1200E 12      0.0    35000.0
  3) 1.0   H       + 1.0   O2       =  1.0   OH      + 1.0   O             0.2200E 15      0.0    16790.0
  4) 1.0   O       + 1.0   H2       =  1.0   OH      + 1.0   H             0.1800E 11      1.0     8900.0
  5) 1.0   H2      + 1.0   OH       =  1.0   H2O     + 1.0   H             0.2200E 14      0.0     5150.0
  6) 1.0   O       + 1.0   H2O      =  2.0   OH      + 0.0                 0.6800E 14      0.0    18360.0
  7) 1.0   H       + 1.0   O2       =  1.0   HO2     + 0.0   M             0.1500E 16      0.0    -1000.0
  8) 0.0   M       + 1.0   O2       =  2.0   O       + 0.0                 0.1800E 19     -1.0   118000.0
  9) 1.0   H       + 1.0   OH       =  1.0   H2O     + 0.0   M             0.8400E 22     -2.0        0.0
 10) 1.0   HO2     + 1.0   NO       =  1.0   NO2     + 1.0   OH            0.1200E 14      0.0     2380.0
 11) 1.0   O       + 1.0   NO2      =  1.0   NO      + 1.0   O2            0.1000E 14      0.0      596.0
 12) 1.0   NO      + 1.0   O        =  1.0   NO2     + 0.0   M             0.5620E 16      0.0    -1160.0
 13) 1.0   NO2     + 1.0   H        =  1.0   NO      + 1.0   OH            0.2900E 15      0.0      795.0
 14) 1.0   O       + 1.0   N2       =  1.0   NO      + 1.0   N             0.7800E 14      0.0    75500.0
 15) 1.0   N       + 1.0   O2       =  1.0   NC      + 1.0   O             0.6400E 10      1.0     6250.0
 16) 1.0   N       + 1.0   OH       =  1.0   NO      + 1.0   H             0.4000E 14      0.0        0.0
 17) 1.0   OH      + 1.0   HO2      =  1.0   H2O     + 1.0   O2            0.5000E 14      0.0     1000.0
 18) 1.0   O       + 1.0   HO2      =  1.0   OH      + 1.0   O2            0.5000E 14      0.0     1000.0
 19) 1.0   H       + 1.0   HO2      =  2.0   OH      + 0.0                 0.2500E 15      0.0     1890.0


THIRD BODY EFFICIENCIES

     1.0   H       + 1.0   O2       =  1.0   HO2     + 0.0   M           O2        2.000  N2         2.000
     1.0   H       + 1.0   O2       =  1.0   HO2     + 0.0   M           H2O      32.500  CO2        7.500
     1.0   H       + 1.0   O2       =  1.0   HO2     + 0.0   M           CO        2.000             0.000
     1.0   H       + 1.0   OH       =  1.0   H2O     + 0.0   M           O2        1.600  H2O       20.000
     1.0   H       + 1.0   OH       =  1.0   H2O     + 0.0   M           CO        1.600  CO2        7.500
     1.0   H       + 1.0   OH       =  1.0   H2O     + 0.0   M           N2        1.600             0.000
KINETIC ORDER OF SPECIES FOR FLOW CALCULATIONS EXCEPT DURING COMBUSTION
 AR            CH4           CO            CO2           H             HO2           H2            H2O
 NH3           N             NO            NO2           N2            O             OH            O2
 C6H6          C7H8          C8H18         AIR

KINETIC ORDER OF SPECIES DURING COMBUSTION AND EXPANSION WITHOUT FLOW
 CO            OH            CO2           H             O2            O             H2            H2O
 HO2           NO            NO2           N2            N             AR            CH4           NH3



AF =  19.749344
                           EFFECTIVE FUEL         EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG       -0.93004913E 02         -0.18318466E 02        -0.21917908E 02

KG-ATOMS/KG                  BOP(I,2)                BOP(I,1)                 BO(I)
             C            0.73581021E-01          0.10891777E-04         0.35565523E-02
             H            0.11530757E 00          0.12245029E-02         0.67226559E-02
             N                0.00000000          0.53321257E-01         0.50751477E-01
             O                0.00000000          0.14938533E-01         0.14218581E-01
             AR               0.00000000          0.31975401E-03         0.30434369E-03

TOTAL COMPUTER TIME=   0.183 SEC         DELTA TIME =  0.183 SEC
```

Excerpts of Intermediate Output

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                  CYCLE   1    LEVEL 1    CASE NO.      512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =   8.5     RPM = 2140.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                     WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                           CAL/MOL           DEG K
FUEL     C  8.00000   H 18.00000                                       0.428571    -59820.961  L     298.15
FUEL     C  7.00000   H  8.00000                                       0.387755      2867.033  L     298.15
FUEL     C  6.00000   H  6.00000                                       0.183673     11718.145  L     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032            *1.000000     -1047.375  G     298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER     RELATIVE HUMIDITY= 0.5500

                    A/F= 19.7493   PERCENT FUEL=    4.8194   EQUIVALENCE RATIO= 0.7367   PHI=   0.7250
FUEL MASS FRACTION = 0.039972                       INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  6.1480
AIR MASS FRACTION = 0.789423                        PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.4434
RESIDUAL MASS FRACTION = 0.170605                   CHEMICAL ENERGY (JOULES/G) =1781.448
RECIRCULATED MASS FRACTION = 0.000000               MASS EFFICIENCY = 0.829395
MASS FRACTION EXHAUST RETAINED = 0.048599            VOLUME EFFICIENCY = 0.815995


THERMODYNAMIC PROPERTIES

STATION                            2         3         4         5         6         7
P, ATM               0.5264    0.5264    0.5264    5.3622    26.577    3.0919    0.9840
T, DEG K              235.6     249.5     238.0     446.6    2164.7    1367.9    1053.8
RHO, G/CC          8.1081-4  7.3990-4  7.9801-4  4.3322-3  4.3322-3  7.9801-4  3.2965-4
H, CAL/G            -54.284   -48.201   -53.246   -1.4839    117.11   -140.02   -234.67
U, CAL/G            -70.006   -65.430   -69.221   -31.459   -31.459   -233.85   -306.96
S, CAL/(G)(K)        1.5676    1.6119    1.5754    1.5754    2.0005    2.0005    2.0005
CP, CAL/(G)(K)       0.2429    0.2424    0.2429    0.2548    0.3544    0.3080    0.2943
GAMMA (S)            1.3787    1.3985    1.3818    1.3578    1.2437    1.2866    1.3040
M, MOL WT            29.782    28.772    29.604    29.604    28.954    28.970    28.970

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR                  0.00000   0.00000   0.00000   0.00000   0.00889   0.00889   0.00889
CO                  0.00000   0.00000   0.00000   0.00000   0.00028   0.00000   0.00000
CO2                 0.00000   0.00000   0.00000   0.00000   0.08518   0.08551   0.08551
H                   0.00000   0.00000   0.00000   0.00000   0.00001   0.00000   0.00000
HO2                 0.00000   0.00000   0.00000   0.00000   0.00001   0.00000   0.00000
H2                  0.00000   0.00000   0.00000   0.00000   0.00005   0.00000   0.00000
H2O                 0.00000   0.00000   0.00000   0.00000   0.08300   0.08378   0.08378
NO                  0.00000   0.00000   0.00000   0.00000   0.00718   0.00718   0.00718
NO2                 0.00000   0.00000   0.00000   0.00000   0.00003   0.00000   0.00000
N2                  0.00000   0.00000   0.00000   0.00000   0.73747   0.73789   0.73789
O                   0.00000   0.00000   0.00000   0.00000   0.00011   0.00000   0.00000
OH                  0.00000   0.00000   0.00000   0.00000   0.00137   0.00001   0.00001
O2                  0.00000   0.00000   0.00000   0.00000   0.07643   0.07673   0.07673
C6H6                0.00337   0.00000   0.00278   0.00278   0.00000   0.00000   0.00000
C7H8                0.00604   0.00000   0.00498   0.00498   0.00000   0.00000   0.00000
C8H18               0.00539   0.00000   0.00444   0.00444   0.00000   0.00000   0.00000
AIR                 0.98520   1.00000   0.98780   0.98780   0.00000   0.00000   0.00000
```

```
STATIONS  1 - 2      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE           0.0000    0.0000    3.6653    6.3684    8.6687    10.745    12.745    14.745    16.745    18.745    20.745    22.745
MASS,G               0.0000    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274    0.0274
VOLUME,CC            0.0000    95.547    96.504    98.431    100.88    103.73    107.04    110.90    115.29    120.21    125.66    131.62
Q, CAL               0.0000    0.0000    0.0711    0.1220    0.1639    0.2007    0.2349    0.2679    0.2996    0.3302    0.3595    0.3875
W, CAL               0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
PUMP W, CAL          0.0000    0.0000    0.0225    0.0667    0.1210    0.1817    0.2492    0.3242    0.4054    0.4912    0.5807    0.6725
DELTA Q/DEL TH       0.0000    0.0198    0.0194    0.0188    0.0182    0.0177    0.0171    0.0165    0.0159    0.0153    0.0146    0.0140
DELTA W/DEL TH       0.0000    0.0000    0.0061    0.0164    0.0236    0.0292    0.0338    0.0375    0.0406    0.0429    0.0447    0.0459

P, ATM               0.5264    0.9840    0.9626    0.9322    0.8981    0.8621    0.8239    0.7835    0.7417    0.6995    0.6575    0.6166
T, DEG K              235.6    1215.1    1200.6    1185.9    1170.9    1155.8    1139.9    1122.9    1105.1    1086.7    1067.9    1048.8
RHO, G/CC          8.1081-4  2.8630-4  2.8346-4  2.7791-4  2.7115-4  2.6370-4  2.5556-4  2.4667-4  2.3727-4  2.2755-4  2.1769-4  2.0784-4
H, CAL/G            -54.284   -266.54   -270.96   -275.44   -279.99   -284.59   -289.40   -294.50   -299.85   -305.37   -311.00   -316.69
U, CAL/G            -70.006   -349.78   -353.20   -356.68   -360.20   -363.76   -367.48   -371.42   -375.55   -379.81   -384.15   -388.53
S, CAL/(G)(K)        1.5676    2.0448    2.0427    2.0411    2.0398    2.0387    2.0376    2.0365    2.0355    2.0345    2.0335    2.0325
CP, CAL/(G)(K)       0.2429    0.3054    0.3047    0.3041    0.3034    0.3027    0.3019    0.3011    0.3002    0.2993    0.2983    0.2974
GAMMA (S)            1.3787    1.2892    1.2900    1.2908    1.2917    1.2925    1.2935    1.2945    1.2956    1.2968    1.2980    1.2993
M, MOL WT            29.782    29.010    29.010    29.010    29.010    29.010    29.010    29.010    29.010    29.010    29.010    29.010

MOLE FRACTIONS

AR                  0.00000   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883
CO2                 0.00000   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317   0.10317
H2O                 0.00000   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748   0.09748
NO                  0.00000   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919   0.00919
N2                  0.00000   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156   0.73156
OH                  0.00000   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006   0.00006
O2                  0.00000   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970   0.04970
C6H6                0.00337   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C7H8                0.00604   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C8H18               0.00539   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
AIR                 0.98520   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
```

```
STATIONS  1 - 2      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE           0.0000    24.745    26.745    27.440
MASS,G               0.0000    0.0274    0.0274    0.0274
VOLUME,CC            0.0000    138.07    145.01    147.53
Q, CAL               0.0000    0.4144    0.4401    0.4488
W, CAL               0.0000    0.0000    0.0000    0.0000
PUMP W, CAL          0.0000    0.7657    0.8594    0.8919
DELTA Q/DEL TH       0.0000    0.0134    0.0129    0.0125
DELTA W/DEL TH       0.0000    0.0466    0.0469    0.0468

P, ATM               0.5264    0.5770    0.5391    0.5264
T, DEG K              235.6    1029.6    1010.4    1003.7
RHO, G/CC          8.1081-4  1.9812-4  1.8864-4  1.8542-4
H, CAL/G            -54.284   -322.39   -328.08   -330.04
U, CAL/G            -70.006   -392.92   -397.28   -398.79
S, CAL/(G)(K)        1.5676    2.0315    2.0306    2.0303
CP, CAL/(G)(K)       0.2429    0.2963    0.2953    0.2950
GAMMA (S)            1.3787    1.3006    1.3020    1.3025
M, MOL WT            29.782    29.010    29.010    29.010

MOLE FRACTIONS

AR                  0.00000   0.00883   0.00883   0.00883
CO2                 0.00000   0.10317   0.10317   0.10317
H2O                 0.00000   0.09748   0.09748   0.09748
NO                  0.00000   0.00919   0.00919   0.00919
N2                  0.00000   0.73156   0.73156   0.73156
OH                  0.00000   0.00006   0.00006   0.00006
O2                  0.00000   0.04970   0.04970   0.04970
C6H6                0.00337   0.00000   0.00000   0.00000
C7H8                0.00604   0.00000   0.00000   0.00000
C8H18               0.00539   0.00000   0.00000   0.00000
AIR                 0.98520   0.00000   0.00000   0.00000

TOTAL COMPUTER TIME=   0.806 SEC        DELTA TIME =   0.083 SEC
```

```
STATIONS  2 - 3     CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE       0.0000   27.440   29.440   31.440   33.440   35.440   37.440   39.440   41.440   43.440   45.440   47.440
MASS,G           0.0000   0.0274   0.0329   0.0388   0.0452   0.0520   0.0591   0.0666   0.0745   0.0827   0.0912   0.1000
VOLUME,CC        0.0000   147.53   155.10   163.13   171.59   180.47   189.75   199.42   209.45   219.84   230.55   241.56
Q, CAL           0.0000   0.4488   0.4709   0.4883   0.5023   0.5137   0.5232   0.5310   0.5376   0.5431   0.5477   0.5515
W, CAL           0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
PUMP W, CAL      0.0000   0.8919   0.9885   1.0907   1.1986   1.3118   1.4301   1.5534   1.6813   1.8137   1.9502   2.0907
DELTA Q/DEL TH   0.0000   0.0125   0.0110   0.0087   0.0070   0.0057   0.0047   0.0039   0.0033   0.0028   0.0023   0.0019
DELTA W/DEL TH   0.0000   0.0468   0.0483   0.0511   0.0539   0.0566   0.0592   0.0616   0.0640   0.0662   0.0683   0.0702

P, ATM           0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264
T, DEG K          235.6   1003.7    881.7    788.0    714.0    654.4    605.7    565.5    531.8    503.3    479.1    458.3
RHO, G/CC      8.1081-4 1.8542-4 2.1200-4 2.3800-4 2.6335-4 2.8792-4 3.1157-4 3.3422-4 3.5579-4 3.7625-4 3.9560-4 4.1385-4
H, CAL/G        -54.284  -330.04  -284.36  -249.58  -222.37  -200.68  -183.10  -168.66  -156.66  -146.59  -138.04  -130.73
U, CAL/G        -70.006  -398.80  -344.49  -303.14  -270.78  -244.96  -224.02  -206.80  -192.49  -180.47  -170.26  -161.53
S, CAL/(G)(K)    1.5676   2.0303   2.0095   1.9775   1.9462   1.9173   1.8911   1.8675   1.8464   1.8275   1.8105   1.7953
CP, CAL/(G)(K)   0.2429   0.2950   0.2883   0.2823   0.2772   0.2728   0.2692   0.2660   0.2634   0.2612   0.2593   0.2577
GAMMA (S)        1.3787   1.3025   1.3099   1.3172   1.3238   1.3298   1.3350   1.3397   1.3437   1.3471   1.3502   1.3528
M, MOL WT        29.782   29.010   29.137   29.234   29.310   29.370   29.420   29.460   29.494   29.522   29.546   29.567

MOLE FRACTIONS

AR              0.00000  0.00883  0.00738  0.00627  0.00540  0.00471  0.00414  0.00368  0.00329  0.00297  0.00270  0.00246
CO2             0.00000  0.10317  0.08621  0.07325  0.06310  0.05499  0.04841  0.04300  0.03850  0.03472  0.03152  0.02877
H2O             0.00000  0.09748  0.08145  0.06921  0.05962  0.05196  0.04574  0.04063  0.03638  0.03281  0.02978  0.02718
NO              0.00000  0.00919  0.00768  0.00652  0.00562  0.00490  0.00431  0.00383  0.00343  0.00309  0.00281  0.00256
N2              0.00000  0.73156  0.61126  0.51942  0.44743  0.38992  0.34327  0.30491  0.27302  0.24621  0.22347  0.20401
OH              0.00000  0.00006  0.00005  0.00005  0.00004  0.00003  0.00003  0.00003  0.00002  0.00002  0.00002  0.00002
O2              0.00000  0.04970  0.04153  0.03529  0.03040  0.02649  0.02332  0.02072  0.01855  0.01673  0.01518  0.01386
C6H6            0.00337  0.00000  0.00055  0.00098  0.00131  0.00158  0.00179  0.00197  0.00212  0.00224  0.00234  0.00243
C7H8            0.00604  0.00000  0.00099  0.00175  0.00235  0.00282  0.00321  0.00352  0.00379  0.00401  0.00420  0.00436
C8H18           0.00539  0.00000  0.00089  0.00156  0.00209  0.00251  0.00286  0.00314  0.00338  0.00357  0.00374  0.00388
AIR             0.98520  0.00000  0.16201  0.28570  0.38264  0.46009  0.52292  0.57457  0.61753  0.65363  0.68425  0.71045
```

```
STATIONS  2 - 3     CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE       0.0000   133.08   142.51   152.51   162.51   172.51   174.51   176.51   178.51   180.00
MASS,G           0.0000   0.4911   0.5153   0.5350   0.5484   0.5556   0.5563   0.5567   0.5569   0.5569
VOLUME,CC        0.0000   728.13   758.59   783.41   800.54   810.03   811.01   811.69   812.07   812.15
Q, CAL           0.0000   0.4570   0.4319   0.4038   0.3748   0.3451   0.3391   0.3331   0.3271   0.3249
W, CAL           0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
PUMP W, CAL      0.0000   8.2934   8.6817   8.9981   9.2165   9.3374   9.3499   9.3586   9.3634   9.3645
DELTA Q/DEL TH   0.0000  -0.0025  -0.0027  -0.0028  -0.0029  -0.0030  -0.0030  -0.0030  -0.0030  -0.0015
DELTA W/DEL TH   0.0000   0.0490   0.0412   0.0316   0.0218   0.0121   0.0063   0.0043   0.0024   0.0007
P, ATM           0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264   0.5264
T, DEG K          235.6    282.9    280.8    279.4    278.5    278.2    278.2    278.2    278.2    278.2
RHO, G/CC      8.1081-4 6.7442-4 6.7933-4 6.8289-4 6.8501-4 6.8585-4 6.8588-4 6.8585-4 6.8578-4 6.8575-4
H, CAL/G        -54.284  -69.656  -68.887  -68.301  -67.907  -67.679  -67.651  -67.630  -67.614  -67.612
U, CAL/G        -70.006  -88.558  -87.652  -86.968  -86.517  -86.266  -86.238  -86.217  -86.203  -86.202
S, CAL/(G)(K)    1.5676   1.6313   1.6288   1.6270   1.6259   1.6254   1.6254   1.6254   1.6254   1.6254
CP, CAL/(G)(K)   0.2429   0.2454   0.2453   0.2452   0.2452   0.2452   0.2452   0.2452   0.2452   0.2452
GAMMA (S)        1.3787   1.3741   1.3743   1.3745   1.3746   1.3746   1.3746   1.3746   1.3746   1.3746
M, MOL WT        29.782   29.738   29.740   29.741   29.742   29.743   29.743   29.743   29.743   29.743

MOLE FRACTIONS

AR              0.00000  0.00050  0.00048  0.00046  0.00045  0.00045  0.00045  0.00044  0.00044  0.00044
CO2             0.00000  0.00589  0.00561  0.00541  0.00528  0.00521  0.00520  0.00520  0.00520  0.00520
H2O             0.00000  0.00557  0.00530  0.00511  0.00499  0.00492  0.00491  0.00491  0.00491  0.00491
NO              0.00000  0.00052  0.00050  0.00048  0.00047  0.00046  0.00046  0.00046  0.00046  0.00046
N2              0.00000  0.04177  0.03981  0.03835  0.03741  0.03693  0.03688  0.03685  0.03684  0.03684
02              0.00000  0.00284  0.00270  0.00261  0.00254  0.00251  0.00251  0.00250  0.00250  0.00250
C6H6            0.00337  0.00318  0.00319  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320
C7H8            0.00604  0.00570  0.00571  0.00572  0.00573  0.00574  0.00574  0.00574  0.00574  0.00574
C8H18           0.00539  0.00508  0.00509  0.00510  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511
AIR             0.98520  0.92894  0.93159  0.93356  0.93481  0.93547  0.93553  0.93557  0.93559  0.93558


TOTAL COMPUTER TIME=   1.179 SEC         DELTA TIME =  0.373 SEC
```

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THE TEMPERATURE=  0.2981E 03 IS OUT OF RANGE FOR POINT     3


STATIONS  3 - 4     CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE         0.0000   180.00   190.00   200.00   210.00   220.00   228.22   235.15   241.14   246.39   251.07   255.28
MASS,G             0.0000   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569
VOLUME,CC          0.0000   812.15   808.36   796.96   777.90   751.14   723.40   696.00   669.52   644.18   620.08   597.22
Q, CAL             0.0000   0.3249   0.2951   0.2656   0.2368   0.2091   0.1876   0.1705   0.1568   0.1456   0.1364   0.1288
W, CAL             0.0000   0.0000  -0.0488  -0.1973  -0.4526  -0.8262  -1.2331  -1.6563  -2.0878  -2.5233  -2.9599  -3.3961
PUMP W, CAL        0.0000   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645
DELTA Q/DEL TH     0.0000  -0.0015  -0.0030  -0.0029  -0.0029  -0.0028  -0.0026  -0.0025  -0.0023  -0.0021  -0.0020  -0.0018
DELTA W/DEL TH     0.0000   0.0000  -0.0049  -0.0149  -0.0255  -0.0374  -0.0495  -0.0610  -0.0721  -0.0829  -0.0934  -0.1037

P, ATM             0.5264   0.5264   0.5304   0.5414   0.5603   0.5885   0.6202   0.6544   0.6905   0.7283   0.7676   0.8084
T, DEG K            235.6    278.2    279.0    280.8    283.7    287.7    292.0    296.4    300.9    305.3    309.8    314.2
RHO, G/CC        8.1081-4 6.8575-4 6.8897-4 6.9882-4 7.1594-4 7.4145-4 7.6989-4 8.0019-4 8.3184-4 8.6456-4 8.9816-4 9.3254-4
H, CAL/G          -54.284  -67.612  -67.418  -66.978  -66.278  -65.288  -64.231  -63.146  -62.048  -60.948  -59.850  -58.758
U, CAL/G          -70.006  -86.202  -86.061  -85.741  -85.231  -84.510  -83.741  -82.950  -82.151  -81.349  -80.548  -79.751
S, CAL/(G)(K)      1.5676   1.6254   1.6256   1.6258   1.6260   1.6262   1.6263   1.6264   1.6265   1.6266   1.6267   1.6267
CP, CAL/(G)(K)     0.2429   0.2452   0.2452   0.2453   0.2455   0.2457   0.2459   0.2462   0.2464   0.2467   0.2469   0.2472
GAMMA (S)          1.3787   1.3746   1.3745   1.3743   1.3740   1.3735   1.3730   1.3725   1.3720   1.3715   1.3709   1.3704
M, MOL WT          29.782   29.743   29.743   29.743   29.743   29.743   29.743   29.743   29.743   29.743   29.743   29.743

MOLE FRACTIONS

AR                0.00000  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044  0.00044
CO2               0.00000  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520  0.00520
H2O               0.00000  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491  0.00491
NO                0.00000  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046  0.00046
N2                0.00000  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684  0.03684
O2                0.00000  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250  0.00250
C6H6              0.00337  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320  0.00320
C7H8              0.00604  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574  0.00574
C8H18             0.00539  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511  0.00511
AIR               0.98520  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558  0.93558



STATIONS  3 - 4     CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE         0.0000   331.08   332.00
MASS,G             0.0000   0.5569   0.5569
VOLUME,CC          0.0000   153.10   149.60
Q, CAL             0.0000   0.2277   0.2339
W, CAL             0.0000  -23.966  -24.406
PUMP W, CAL        0.0000   9.3645   9.3645
DELTA Q/DEL TH     0.0000   0.0066   0.0068
DELTA W/DEL TH     0.0000  -0.4743  -0.4773

P, ATM             0.5264   5.1229   5.2837
T, DEG K            235.6    510.5    514.5
RHO, G/CC        8.1081-4 3.6376-3 3.7226-3
H, CAL/G          -54.284   -8.8856  -7.8382
U, CAL/G          -70.006  -42.991  -42.211
S, CAL/(G)(K)      1.5676   1.6264   1.6263
CP, CAL/(G)(K)     0.2429   0.2618   0.2621
GAMMA (S)          1.3787   1.3427   1.3422
M, MOL WT          29.782   29.743   29.743

MOLE FRACTIONS

AR                0.00000  0.00044  0.00044
CO2               0.00000  0.00520  0.00520
H2O               0.00000  0.00491  0.00491
NO                0.00000  0.00046  0.00046
N2                0.00000  0.03684  0.03684
O2                0.00000  0.00250  0.00250
C6H6              0.00337  0.00320  0.00320
C7H8              0.00604  0.00574  0.00574
C8H18             0.00539  0.00511  0.00511
AIR               0.98520  0.93558  0.93558

TOTAL COMPUTER TIME=    1.454 SEC         DELTA TIME =   0.275 SEC
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STATIONS  4 - 5     CYCLE 1

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =     0.0000 SEC    BETA =   0.000

BURNED - UNBURNED ALTERNATELY

EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE          0.0000    332.00    332.00    332.18    332.18    332.62    332.62    333.24    333.24    334.00    334.00    334.94    334.94
MASS,G              0.0000    0.0001    0.5568    0.0001    0.5568    0.0001    0.5568    0.0003    0.5566    0.0007    0.5561    0.0016    0.5553
VOLUME,CC           0.0000    0.0605    149.54    0.0662    148.88    0.1312    147.17    0.3394    144.71    0.7635    141.62    1.5349    137.61
Q, CAL              0.0000    0.2339    0.2339    0.2352    0.2352    0.2382    0.2382    0.2427    0.2427    0.2482    0.2482    0.2557    0.2557
W, CAL              0.0000   -24.406   -24.406   -24.491   -24.491   -24.704   -24.704   -25.001   -25.001   -25.363   -25.363   -25.817   -25.817
PUMP W, CAL         0.0000    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645
DELTA Q/DEL TH      0.0000    0.0000    0.0068    0.0000    0.0069    0.0000    0.0069    0.0001    0.0071    0.0002    0.0073    0.0004    0.0076
DELTA W/DEL TH      0.0000   -0.0002   -0.4778    0.0041   -0.4822    0.0190   -0.4976    0.0444   -0.5237    0.0765   -0.5569    0.1150   -0.5970
MB/M, MU/M          0.0000    0.0001    0.9999    0.0001    0.9999    0.0002    0.9998    0.0005    0.9994    0.0013    0.9987    0.0028    0.997_
VB/V, VU/V          0.0000    0.0004    0.9996    0.0004    0.9996    0.0009    0.9991    0.0023    0.9977    0.0054    0.9946    0.0110    0.9890

P, ATM              0.5264    5.2837    5.2837    5.3165    5.3165    5.3982    5.3982    5.5185    5.5185    5.6744    5.6744    5.8852    5.8852
T, DEG K             235.6    2029.2     514.5    2031.3     515.2    2035.0     517.2    2038.6     520.1    2043.5     523.8    2050.2     528.6
RHO, G/CC         8.1081-4  9.2009-4  3.7226-3  9.2486-4  3.7401-3  9.3732-4  3.7830-3  9.5652-4  3.8459-3  9.8121-4  3.9269-3  1.0143-3  4.0356-3
H, CAL/G           -54.284   -7.8386   -7.8383   -7.1086   -7.6353   -5.8037   -7.1153   -4.5431   -6.3590   -2.8614   -5.3970   -0.4952   -4.1274
U, CAL/G           -70.006   -146.91   -42.211   -146.32   -42.060   -145.27   -41.672   -144.26   -41.109   -142.91   -40.391   -141.01   -39.444
S, CAL/(G)(K)       1.5676    2.0926    1.6263    2.0925    1.6263    2.0921    1.6263    2.0912    1.6263    2.0901    1.6263    2.0888    1.6263
CP, CAL/(G)(K)      0.2429    0.3535    0.2621    0.3537    0.2621    0.3540    0.2623    0.3543    0.2626    0.3547    0.2629    0.3553    0.2633
GAMMA (S)           1.3787    1.2441    1.3422    1.2440    1.3420    1.2438    1.3418    1.2436    1.3413    1.2433    1.3408    1.2429    1.3401
M, MOL WT           29.782    28.996    29.743    28.996    29.743    28.995    29.743    28.995    29.743    28.995    29.743    28.994    29.743

MOLE FRACTIONS

AR                 0.00000   0.00882   0.00044   0.00882   0.00044   0.00882   0.00044   0.00882   0.00044   0.00882   0.00044   0.00882   0.00044
CO                 0.00000   0.00033   0.00000   0.00033   0.00000   0.00034   0.00000   0.00034   0.00000   0.00035   0.00000   0.00037   0.00000
CO2                0.00000   0.10280   0.00520   0.10279   0.00520   0.10279   0.00520   0.10278   0.00520   0.10277   0.00520   0.10275   0.00520
H                  0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000
H2                 0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000
H2O                0.00000   0.09684   0.00491   0.09684   0.00491   0.09683   0.00491   0.09682   0.00491   0.09681   0.00491   0.09679   0.00491
NO                 0.00000   0.00422   0.00046   0.00424   0.00046   0.00429   0.00046   0.00433   0.00046   0.00438   0.00046   0.00446   0.00046
NO2                0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000
N2                 0.00000   0.73368   0.03684   0.73366   0.03684   0.73363   0.03684   0.73361   0.03684   0.73357   0.03684   0.73352   0.03684
O                  0.00000   0.00008   0.00000   0.00008   0.00000   0.00009   0.00000   0.00009   0.00000   0.00009   0.00000   0.00009   0.00000
OH                 0.00000   0.00110   0.00000   0.00111   0.00000   0.00112   0.00000   0.00114   0.00000   0.00116   0.00000   0.00118   0.00000
O2                 0.00000   0.05204   0.00250   0.05203   0.00250   0.05201   0.00250   0.05199   0.00250   0.05196   0.00250   0.05192   0.00250
C6H6               0.00337   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320
C7H8               0.00604   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574
C8H18              0.00539   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511
AIR                0.98520   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558
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STATIONS  4 - 5      CYCLE 1

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000

BURNED - UNBURNED ALTERNATELY

EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE         0.0000    405.68    405.68    409.63    409.63    413.44    413.44    417.11    417.11    420.23    420.23
MASS,G             0.0000    0.5180    0.0389    0.5354    0.0215    0.5475    0.0094    0.5545    0.0024    0.5568    0.0001
VOLUME,CC          0.0000    226.64    5.2299    250.88    3.0785    274.84    1.4353    298.12    0.3867    317.92    0.0097
Q, CAL             0.0000    9.7400    9.7400    10.864    10.864    11.966    11.966    13.023    13.023    13.909    13.909
W, CAL             0.0000    21.035    21.035    27.725    27.725    33.923    33.923    39.576    39.576    44.119    44.119
PUMP W, CAL        0.0000    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645
DELTA Q/DEL TH     0.0000    0.2801    0.0020    0.2860    0.0010    0.2876    0.0004    0.2851    0.0001    0.2797    0.0000
DELTA W/DEL TH     0.0000    1.9520   -0.2053    1.8586   -0.1630    1.7431   -0.1181    1.6131   -0.0718    1.4830   -0.0279
MB/M, MU/M         0.0000    0.9302    0.0698    0.9615    0.0385    0.9832    0.0168    0.9958    0.0042    0.9999    0.0001
VB/V, VU/V         0.0000    0.9774    0.0226    0.9879    0.0121    0.9948    0.0052    0.9987    0.0013    1.0000    0.0000

P, ATM             0.5264    13.064    13.064    11.976    11.976    10.968    10.968    10.042    10.042    9.2890    9.2890
T, DEG K            235.6    2020.0     637.2    1983.3     622.9    1946.1     608.7    1908.5     594.8    1874.8     582.9
RHO, G/CC        8.1081-4  2.2856-3  7.4309-3  2.1342-3  6.9690-3  1.9921-3  6.5312-3  1.8600-3  6.1194-3  1.7515-3  5.7764-3
H, CAL/G          -54.284   -11.724    24.966   -24.417    21.068   -37.172    17.232   -49.986    13.497   -61.410    10.287
U, CAL/G          -70.006   -150.14   -17.608   -160.31   -20.548   -170.51   -23.437   -180.74   -26.246   -189.85   -28.656
S, CAL/(G)(K)      1.5676    2.0286    1.6230    2.0282    1.6226    2.0277    1.6223    2.0271    1.6220    2.0264    1.6217
CP, CAL/(G)(K)     0.2429    0.3481    0.2724    0.3454    0.2712    0.3427    0.2700    0.3402    0.2688    0.3381    0.2678
GAMMA (S)          1.3787    1.2475    1.3249    1.2496    1.3269    1.2516    1.3288    1.2535    1.3307    1.2553    1.3324
M, MOL WT          29.782    29.001    29.743    29.002    29.743    29.004    29.743    29.005    29.743    29.006    29.743

MOLE FRACTIONS

AR                0.00000   0.00883   0.00044   0.00883   0.00044   0.00883   0.00044   0.00883   0.00044   0.00883   0.00044
CO                0.00000   0.00019   0.00000   0.00015   0.00000   0.00011   0.00000   0.00008   0.00000   0.00006   0.00000
CO2               0.00000   0.10295   0.00520   0.10300   0.00520   0.10304   0.00520   0.10308   0.00520   0.10310   0.00520
H2                0.00000   0.00004   0.00000   0.00003   0.00000   0.00002   0.00000   0.00002   0.00000   0.00001   0.00000
H2O               0.00000   0.09702   0.00491   0.09709   0.00491   0.09716   0.00491   0.09722   0.00491   0.09727   0.00491
NO                0.00000   0.00412   0.00046   0.00374   0.00046   0.00337   0.00046   0.00303   0.00046   0.00274   0.00046
NO2               0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000
N2                0.00000   0.73385   0.03684   0.73408   0.03684   0.73431   0.03684   0.73451   0.03684   0.73468   0.03684
O                 0.00000   0.00005   0.00000   0.00004   0.00000   0.00003   0.00000   0.00002   0.00000   0.00002   0.00000
OH                0.00000   0.00084   0.00000   0.00072   0.00000   0.00061   0.00000   0.00051   0.00000   0.00043   0.00000
O2                0.00000   0.05210   0.00250   0.05230   0.00250   0.05250   0.00250   0.05269   0.00250   0.05284   0.00250
C6H6              0.00337   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320   0.00000   0.00320
C7H8              0.00604   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574   0.00000   0.00574
C8H18             0.00539   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511   0.00000   0.00511
AIR               0.98520   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558   0.00000   0.93558

TOTAL COMPUTER TIME=   2.734 SEC        DELTA TIME =  1.280 SEC
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STATIONS  5 - 6      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT

CRANKANGLE       0.0000   420.23   422.23   424.23   426.23   428.23   430.23   432.23   434.23   436.23   438.23   440.23
MASS,G           0.0000   0.5568   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569   0.5569
VOLUME,CC        0.0000   317.92   330.56   343.32   356.19   369.14   382.15   395.21   408.29   421.37   434.42   447.45
Q, CAL           0.0000   13.909   14.464   15.009   15.545   16.072   16.592   17.103   17.606   18.103   18.592   19.075
W, CAL           0.0000   44.119   46.889   49.550   52.103   54.553   56.903   59.157   61.317   63.387   65.371   67.271
PUMP W, CAL      0.0000   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645   9.3645
DELTA Q/DEL TH   0.0000   0.2797   0.2774   0.2726   0.2681   0.2637   0.2596   0.2556   0.2518   0.2481   0.2447   0.2413
DELTA W/DEL TH   0.0000   1.4131   1.3851   1.3301   1.2768   1.2251   1.1751   1.1267   1.0801   1.0351   0.9917   0.9499

P, ATM           0.5264   9.2890   8.8253   8.3960   7.9983   7.6296   7.2876   6.9700   6.6750   6.4006   6.1452   5.9073
T, DEG K          235.6   1874.8   1852.0   1829.9   1808.6   1788.0   1768.1   1748.8   1730.2   1712.3   1694.9   1678.1
RHO, G/CC      8.1081-4 1.7515-3 1.6845-3 1.6219-3 1.5633-3 1.5085-3 1.4571-3 1.4090-3 1.3638-3 1.3215-3 1.2818-3 1.2445-3
H, CAL/G        -54.284  -61.410  -68.944  -76.212  -83.222  -89.983  -96.501  -102.79  -108.84  -114.69  -120.32  -125.74
U, CAL/G        -70.006  -189.85  -195.82  -201.57  -207.12  -212.47  -217.62  -222.59  -227.37  -231.98  -236.42  -240.70
S, CAL/(G)(K)    1.5676   2.0264   2.0259   2.0254   2.0248   2.0243   2.0238   2.0233   2.0228   2.0222   2.0217   2.0212
CP, CAL/(G)(K)   0.2429   0.3381   0.3308   0.3298   0.3288   0.3279   0.3271   0.3263   0.3255   0.3248   0.3242   0.3235
GAMMA (S)        1.3787   1.2553   1.2622   1.2631   1.2640   1.2648   1.2656   1.2663   1.2670   1.2677   1.2683   1.2690
M, MOL WT        29.782   29.006   29.007   29.007   29.008   29.008   29.008   29.009   29.009   29.009   29.009   29.010

MOLE FRACTIONS

AR              0.00000  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883
CO              0.00000  0.00006  0.00005  0.00004  0.00004  0.00003  0.00002  0.00002  0.00002  0.00001  0.00001  0.00001
CO2             0.00000  0.10310  0.10311  0.10312  0.10313  0.10314  0.10315  0.10315  0.10316  0.10316  0.10316  0.10316
H2              0.00000  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00000  0.00000  0.00000  0.00000
H2O             0.00000  0.09727  0.09729  0.09732  0.09734  0.09736  0.09738  0.09739  0.09740  0.09742  0.09743  0.09744
NO              0.00000  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274  0.00274
NO2             0.00000  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001
N2              0.00000  0.73468  0.73470  0.73471  0.73472  0.73473  0.73474  0.73475  0.73475  0.73476  0.73476  0.73477
O               0.00000  0.00002  0.00002  0.00001  0.00001  0.00001  0.00001  0.00001  0.00001  0.00000  0.00000  0.00000
OH              0.00000  0.00043  0.00039  0.00035  0.00031  0.00028  0.00025  0.00022  0.00020  0.00018  0.00016  0.00014
O2              0.00000  0.05284  0.05285  0.05286  0.05287  0.05287  0.05288  0.05289  0.05289  0.05289  0.05290  0.05290
C6H6            0.00337  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
C7H8            0.00604  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
C8H18           0.00539  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
AIR             0.98520  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
```

```
STATIONS  5 - 6      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE           0.0000    496.44    500.93    505.94    511.62    518.27    526.48    536.48    540.00
MASS,G               0.0000    0.5569    0.5569    0.5569    0.5569    0.5569    0.5569    0.5569    0.5569
VOLUME,CC            0.0000    739.76    753.95    767.96    781.51    794.21    805.21    811.68    812.15
Q, CAL               0.0000    30.679    31.490    32.379    33.372    34.512    35.892    37.535    38.103
W, CAL               0.0000    96.692    97.691    98.648    99.549    100.37    101.07    101.47    101.49
PUMP W, CAL          0.0000    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645    9.3645
DELTA Q/DEL TH       0.0000    0.1833    0.1806    0.1777    0.1747    0.1715    0.1681    0.1643    0.1613
DELTA W/DEL TH       0.0000    0.2526    0.2224    0.1912    0.1586    0.1236    0.0846    0.0400    0.0081

P, ATM               0.5264    2.9440    2.8607    2.7806    2.7041    2.6320    2.5658    2.5158    2.5057
T, DEG K              235.6    1382.8    1369.4    1355.8    1341.8    1327.2    1311.8    1296.5    1292.1
RHO, G/CC          8.1081-4  7.5272-4  7.3854-4  7.2507-4  7.1250-4  7.0111-4  6.9152-4  6.8601-4  6.8562-4
H, CAL/G            -54.284   -219.65   -223.81   -228.07   -232.43   -236.95   -241.73   -246.44   -247.82
U, CAL/G            -70.006   -314.37   -317.62   -320.94   -324.34   -327.86   -331.59   -335.25   -336.32
S, CAL/(G)(K)        1.5676    2.0074    2.0063    2.0052    2.0038    2.0023    2.0004    1.9982    1.9974
CP, CAL/(G)(K)       0.2429    0.3124    0.3119    0.3113    0.3108    0.3102    0.3096    0.3089    0.3087
GAMMA (S)            1.3787    1.2809    1.2815    1.2821    1.2827    1.2834    1.2842    1.2849    1.2851
M, MOL WT            29.782    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011

MOLE FRACTIONS

AR                  0.00000   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883
CO2                 0.00000   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318
H2O                 0.00000   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751
NO                  0.00000   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274
N2                  0.00000   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480
OH                  0.00000   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001
O2                  0.00000   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294
C6H6                0.00337   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C7H8                0.00604   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C8H18               0.00539   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
AIR                 0.98520   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000


TOTAL COMPUTER TIME=    3.561 SEC          DELTA TIME =  0.827 SEC

THE TEMPERATURE=  0.2981E 03 IS OUT OF RANGE FOR POINT   15
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STATIONS  7 - 8      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE           0.0000    540.00    550.00    560.00    570.00    580.00    590.00    600.00    610.00    620.00    630.00    640.00
MASS,G               0.0000    0.2702    0.2710    0.2693    0.2648    0.2577    0.2477    0.2350    0.2195    0.2016    0.1816    0.1600
VOLUME,CC            0.0000    812.15    808.36    796.96    777.90    751.14    716.71    674.76    625.72    570.36    509.87    445.93
Q, CAL               0.0000    38.103    38.762    39.405    40.028    40.625    41.192    41.726    42.221    42.676    43.086    43.452
W, CAL               0.0000    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49
PUMP W, CAL          0.0000    9.3645    9.2741    9.0024    8.5483    7.9106    7.0900    6.0904    4.9219    3.6027    2.1613    0.6374
DELTA Q/DEL TH       0.0000    0.0665    0.0659    0.0643    0.0623    0.0597    0.0567    0.0533    0.0496    0.0454    0.0411    0.0366
DELTA W/DEL TH       0.0000    0.0000   -0.0090   -0.0272   -0.0454   -0.0638   -0.0821   -0.1000   -0.1169   -0.1319   -0.1441   -0.1524

P, ATM               0.5264    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840
T, DEG K              235.6    1045.9    1037.7    1029.7    1021.8    1014.1    1006.5     999.0     991.6     984.3     977.0     969.7
RHO, G/CC          8.1081-4  3.3261-4  3.3524-4  3.3785-4  3.4045-4  3.4305-4  3.4564-4  3.4823-4  3.5083-4  3.5345-4  3.5609-4  3.5877-4
H, CAL/G            -54.284   -322.44   -324.87   -327.25   -329.59   -331.87   -334.12   -336.33   -338.51   -340.66   -342.81   -344.95
U, CAL/G            -70.006   -394.08   -395.96   -397.79   -399.58   -401.34   -403.06   -404.76   -406.43   -408.09   -409.73   -411.37
S, CAL/(G)(K)        1.5676    1.9974    1.9950    1.9927    1.9905    1.9882    1.9860    1.9838    1.9816    1.9794    1.9772    1.9750
CP, CAL/(G)(K)       0.2429    0.2972    0.2968    0.2963    0.2959    0.2955    0.2951    0.2947    0.2943    0.2938    0.2934    0.2930
GAMMA (S)            1.3787    1.2995    1.3001    1.3006    1.3012    1.3017    1.3023    1.3028    1.3034    1.3040    1.3045    1.3051
M, MOL WT            29.782    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011

MOLE FRACTIONS

AR                  0.00000   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883
CO2                 0.00000   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318
H2O                 0.00000   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751
NO                  0.00000   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274
N2                  0.00000   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480
OH                  0.00000   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001
O2                  0.00000   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294
C6H6                0.00337   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C7H8                0.00604   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C8H18               0.00539   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
AIR                 0.98520   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
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STATIONS  7 - 8      CYCLE 1
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE         0.0000    650.00    660.00    670.00    680.00    690.00    700.00    710.00    720.00    0.0000
MASS,G             0.0000    0.1376    0.1153    0.0941    0.0749    0.0588    0.0467    0.0392    0.0369   -0.5200
VOLUME,CC          0.0000    380.63    316.46    256.08    202.19    157.30    123.57    102.64    95.547    0.0000
Q, CAL             0.0000    43.772    44.048    44.282    44.479    44.644    44.783    44.905    45.016    42.676
W, CAL             0.0000    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49    101.49
PUMP W, CAL        0.0000   -0.9186   -2.4478   -3.8866   -5.1707   -6.2404   -7.0443   -7.5430   -7.7120    3.6027
DELTA Q/DEL TH     0.0000    0.0320    0.0276    0.0234    0.0197    0.0165    0.0139    0.0121    0.0111    0.0000
DELTA W/DEL TH     0.0000   -0.1556   -0.1529   -0.1439   -0.1284   -0.1070   -0.0804   -0.0499   -0.0169    0.0000

P, ATM             0.5264    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840    0.9840
T, DEG K            235.6     962.3     954.8     947.2     939.1     930.6     921.5     911.7     901.6    1009.5
RHO, G/CC        8.1081-4  3.6151-4  3.6434-4  3.6729-4  3.7043-4  3.7382-4  3.7753-4  3.8158-4  3.8585-4  3.4463-4
H, CAL/G          -54.284   -347.10   -349.28   -351.53   -353.86   -356.34   -359.00   -361.83   -364.75   -333.25
U, CAL/G          -70.006   -413.02   -414.69   -416.41   -418.19   -420.09   -422.12   -424.28   -426.51   -402.39
S, CAL/(G)(K)      1.5676    1.9728    1.9705    1.9682    1.9657    1.9630    1.9602    1.9571    1.9539    1.9869
CP, CAL/(G)(K)     0.2429    0.2926    0.2921    0.2917    0.2912    0.2906    0.2901    0.2895    0.2888    0.2953
GAMMA (S)          1.3787    1.3057    1.3063    1.3070    1.3076    1.3084    1.3091    1.3100    1.3109    1.3021
M, MOL WT          29.782    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011    29.011

MOLE FRACTIONS

AR                0.00000   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883   0.00883
CO2               0.00000   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318   0.10318
H2O               0.00000   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751   0.09751
NO                0.00000   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274   0.00274
N2                0.00000   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480   0.73480
OH                0.00000   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001   0.00001
O2                0.00000   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294   0.05294
C6H6              0.00337   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C7H8              0.00604   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
C8H18             0.00539   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
AIR               0.98520   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000


TOTAL COMPUTER TIME=   3.683 SEC        DELTA TIME =  0.122 SEC
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STATIONS  3 - 4      CYCLE 4
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE         0.0000    313.23    315.23    317.23    319.23    321.23    323.23    325.23    327.23    329.23    331.23    332.00
MASS,G             0.0000    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673    0.5673
VOLUME,CC          0.0000    237.84    226.92    216.32    206.05    196.14    186.60    177.45    168.71    160.39    152.52    149.60
Q, CAL             0.0000   -0.1765   -0.1704   -0.1637   -0.1562   -0.1480   -0.1391   -0.1293   -0.1186   -0.1070   -0.0945   -0.0895
W, CAL             0.0000   -16.219   -16.994   -17.797   -18.626   -19.481   -20.361   -21.264   -22.187   -23.126   -24.078   -24.447
PUMP W, CAL        0.0000    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761
DELTA Q/DEL TH     0.0000    0.0027    0.0030    0.0034    0.0037    0.0041    0.0045    0.0049    0.0053    0.0058    0.0063    0.0064
DELTA W/DEL TH     0.0000   -0.3736   -0.3874   -0.4012   -0.4146   -0.4277   -0.4400   -0.4514   -0.4614   -0.4698   -0.4759   -0.4788

P, ATM             0.5264    2.8395    3.0257    3.2275    3.4463    3.6831    3.9388    4.2143    4.5102    4.8266    5.1635    5.2985
T, DEG K            235.6     431.3     438.5     445.9     453.5     461.3     469.4     477.6     485.9     494.4     502.9     506.2
RHO, G/CC        8.1081-4  2.3854-3  2.5001-3  2.6227-3  2.7534-3  2.8925-3  3.0405-3  3.1972-3  3.3629-3  3.5373-3  3.7199-3  3.7923-3
H, CAL/G          -54.284   -37.688   -35.853   -33.956   -31.997   -29.980   -27.908   -25.786   -23.620   -21.418   -19.191   -18.329
U, CAL/G          -70.006   -66.516   -65.160   -63.758   -62.309   -60.816   -59.281   -57.707   -56.099   -54.463   -52.807   -52.166
S, CAL/(G)(K)      1.5676    1.6265    1.6265    1.6265    1.6265    1.6264    1.6264    1.6264    1.6263    1.6263    1.6262    1.6262
CP, CAL/(G)(K)     0.2429    0.2554    0.2560    0.2565    0.2571    0.2578    0.2584    0.2591    0.2597    0.2604    0.2611    0.2614
GAMMA (S)          1.3787    1.3545    1.3534    1.3524    1.3513    1.3501    1.3489    1.3477    1.3465    1.3453    1.3440    1.3436
M, MOL WT          29.782    29.730    29.730    29.730    29.730    29.730    29.730    29.730    29.730    29.730    29.730    29.730

MOLE FRACTIONS

AR                0.00000   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059   0.00059
CO2               0.00000   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695   0.00695
H2O               0.00000   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657   0.00657
NO                0.00000   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017   0.00017
N2                0.00000   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948   0.04948
O2                0.00000   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357   0.00357
C6H6              0.00337   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315   0.00315
C7H8              0.00604   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563   0.00563
C8H18             0.00539   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502   0.00502
AIR               0.98520   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887   0.91887


TOTAL COMPUTER TIME=  10.671 SEC        DELTA TIME =  0.242 SEC
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STATIONS  4 - 5     CYCLE 4

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =     0.0000 SEC    BETA =   0.000

BURNED - UNBURNED ALTERNATELY

EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE        0.0000    332.00    332.00    332.19    332.19    332.76    332.76    333.63    333.63    336.40    336.40    341.13    341.13
MASS,G            0.0000    0.0001    0.5672    0.0001    0.5672    0.0002    0.5671    0.0005    0.5668    0.0035    0.5638    0.0147    0.5526
VOLUME,CC         0.0000    0.0606    149.54    0.0668    148.84    0.1656    146.64    0.5369    143.13    3.2059    131.09    11.142    109.41
Q, CAL            0.0000   -0.0895   -0.0895   -0.0883   -0.0883   -0.0846   -0.0846   -0.0787   -0.0787   -0.0574   -0.0574   -0.0060   -0.0060
W, CAL            0.0000   -24.447   -24.447   -24.536   -24.536   -24.811   -24.811   -25.231   -25.231   -26.574   -26.574   -28.889   -28.889
PUMP W, CAL       0.0000    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761
DELTA Q/DEL TH    0.0000    0.0000    0.0064    0.0000    0.0064    0.0000    0.0065    0.0001    0.0067    0.0005    0.0072    0.0024    0.0085
DELTA W/DEL TH    0.0000   -0.0002   -0.4791    0.0043   -0.4838    0.0226   -0.5026    0.0569   -0.5380    0.1392   -0.6237    0.2860   -0.7763
MB/M, MU/M        0.0000    0.0001    0.9999    0.0001    0.9999    0.0003    0.9997    0.0009    0.9991    0.0062    0.9938    0.0259    0.9741
VB/V, VU/V        0.0000    0.0004    0.9996    0.0004    0.9996    0.0011    0.9989    0.0037    0.9963    0.0239    0.9761    0.0924    0.9076

P, ATM            0.5264    5.2985    5.2985    5.3329    5.3329    5.4393    5.4393    5.6139    5.6139    6.2692    6.2692    7.7689    7.7689
T, DEG K           235.6    1999.4     506.2    2001.7     507.0    2006.3     509.6    2012.0     513.6    2033.9     528.1    2078.8     557.3
RHO, G/CC      8.1081-4  9.3652-4  3.7923-3  9.4149-4  3.8109-3  9.5807-4  3.8675-3  9.8603-4  3.9599-3  1.0892-3  4.3007-3  1.3205-3  5.0507-3
H, CAL/G         -54.284   -18.330   -18.329   -17.560   -18.120   -16.021   -17.455   -14.098   -16.385   -6.6461   -12.577    8.8239   -4.8686
U, CAL/G         -70.006   -155.34   -52.166   -154.73   -52.009   -153.51   -51.515   -151.98   -50.718   -146.03   -47.879   -133.66   -42.11
S, CAL/(G)(K)     1.5676    2.0872    1.6262    2.0871    1.6262    2.0865    1.6262    2.0853    1.6262    2.0814    1.6261    2.0743    1.6260
CP, CAL/(G)(K)    0.2429    0.3501    0.2614    0.3293    0.2615    0.3294    0.2617    0.3295    0.2620    0.3299    0.2632    0.3307    0.2657
GAMMA (S)         1.3787    1.2464    1.3436    1.2628    1.3434    1.2627    1.3431    1.2626    1.3425    1.2622    1.3404    1.2614    1.3362
M, MOL WT         29.782    28.998    29.730    28.998    29.730    28.998    29.730    28.998    29.730    28.997    29.730    28.994    29.730

MOLE FRACTIONS

AR               0.00000   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00882   0.00059
CO               0.00000   0.00025   0.00000   0.00025   0.00000   0.00026   0.00000   0.00026   0.00000   0.00029   0.00000   0.00037   0.00000
CO2              0.00000   0.10288   0.00695   0.10288   0.00695   0.10288   0.00695   0.10287   0.00695   0.10284   0.00695   0.10275   0.00695
H                0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000
H2               0.00000   0.00005   0.00000   0.00005   0.00000   0.00005   0.00000   0.00005   0.00000   0.00006   0.00000   0.00007   0.00000
H2O              0.00000   0.09694   0.00657   0.09694   0.00657   0.09693   0.00657   0.09692   0.00657   0.09688   0.00657   0.09677   0.00657
NO               0.00000   0.00390   0.00017   0.00391   0.00017   0.00392   0.00017   0.00394   0.00017   0.00402   0.00017   0.00417   0.00017
NO2              0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000   0.00001   0.00000
N2               0.00000   0.73390   0.04948   0.73390   0.04948   0.73389   0.04948   0.73387   0.04948   0.73381   0.04948   0.73366   0.04948
O                0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00007   0.00000   0.00009   0.00000
OH               0.00000   0.00095   0.00000   0.00096   0.00000   0.00097   0.00000   0.00098   0.00000   0.00105   0.00000   0.00123   0.00000
O2               0.00000   0.05221   0.00357   0.05221   0.00357   0.05220   0.00357   0.05219   0.00357   0.05214   0.00357   0.05206   0.00357
C6H6             0.00337   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315
C7H8             0.00604   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563
C8H18            0.00539   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502
AIR              0.98520   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887
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STATIONS  4 - 5     CYCLE 4

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG     COSINE  COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000

BURNED - UNBURNED ALTERNATELY

EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE          0.0000    398.19    398.19    402.66    402.66    406.96    406.96    411.96    411.96    416.49    416.49    420.23    420.23
MASS,G              0.0000    0.4813    0.0860    0.5108    0.0564    0.5340    0.0333    0.5535    0.0137    0.5640    0.0033    0.5672    0.0001
VOLUME,CC           0.0000    183.25    10.096    208.65    7.0831    234.42    4.4759    265.50    2.0075    294.17    0.5205    317.92    0.0096
Q, CAL              0.0000    7.2030    7.2030    8.3756    8.3756    9.5493    9.5493    10.943    10.943    12.206    12.206    13.233    13.233
W, CAL              0.0000    7.9898    7.9898    15.905    15.905    23.386    23.386    31.727    31.727    38.821    38.821    44.300    44.300
PUMP W, CAL         0.0000    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761    9.3761
DELTA Q/DEL TH      0.0000    0.2429    0.0053    0.2592    0.0035    0.2706    0.0021    0.2775    0.0010    0.2786    0.0003    0.2743    0.0001
DELTA W/DEL TH      0.0000    2.0471   -0.2777    2.0107   -0.2373    1.9338   -0.1956    1.8110   -0.1440    1.6532   -0.0859    1.4960   -0.0323
MB/M, MU/M          0.0000    0.8484    0.1516    0.9005    0.0995    0.9413    0.0587    0.9758    0.0242    0.9942    0.0058    0.9999    0.0001
VB/V, VU/V          0.0000    0.9478    0.0522    0.9672    0.0328    0.9813    0.0187    0.9925    0.0075    0.9982    0.0018    1.0000    0.0000

P, ATM              0.5264    15.270    15.270    13.959    13.959    12.731    12.731    11.367    11.367    10.202    10.202    9.2895    9.2895
T, DEG K             235.6    2054.6     649.7    2015.0     634.6    1975.4     619.6    1927.2     601.5    1881.0     584.8    1840.5     570.7
RHO, G/CC         8.1081-4  2.6265-3  8.5157-3  2.4484-3  7.9691-3  2.2778-3  7.4445-3  2.0849-3  6.8465-3  1.9172-3  6.3206-3  1.7842-3  5.8977-3
H, CAL/G           -54.284    0.9203    20.033   -12.518    15.931   -25.882    11.842   -42.036    6.9692   -57.397    2.4735   -70.801   -1.3055
U, CAL/G           -70.006   -139.87   -23.392   -150.59   -26.489   -161.23   -29.572   -174.07   -33.239   -186.27   -36.616   -196.89   -39.450
S, CAL/(G)(K)       1.5676    2.0241    1.6221    2.0237    1.6217    2.0233    1.6214    2.0228    1.6210    2.0221    1.6206    2.0213    1.6203
CP, CAL/(G)(K)      0.2429    0.3303    0.2734    0.3296    0.2722    0.3288    0.2709    0.3278    0.2694    0.3268    0.2680    0.3259    0.2668
GAMMA (S)           1.3787    1.2618    1.3235    1.2625    1.3255    1.2633    1.3275    1.2642    1.3300    1.2652    1.3323    1.2662    1.3343
M, MOL WT           29.782    28.999    29.730    29.001    29.730    29.003    29.730    29.005    29.730    29.006    29.730    29.007    29.730

MOLE FRACTIONS

AR                 0.00000   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059   0.00883   0.00059
CO                 0.00000   0.00024   0.00000   0.00018   0.00000   0.00014   0.00000   0.00010   0.00000   0.00007   0.00000   0.00005   0.00000
CO2                0.00000   0.10290   0.00695   0.10296   0.00695   0.10301   0.00695   0.10306   0.00695   0.10309   0.00695   0.10312   0.00695
H2                 0.00000   0.00005   0.00000   0.00004   0.00000   0.00003   0.00000   0.00002   0.00000   0.00002   0.00000   0.00001   0.00000
H2O                0.00000   0.09695   0.00657   0.09704   0.00657   0.09711   0.00657   0.09719   0.00657   0.09726   0.00657   0.09731   0.00657
NO                 0.00000   0.00539   0.00017   0.00537   0.00017   0.00535   0.00017   0.00533   0.00017   0.00532   0.00017   0.00531   0.00017
NO2                0.00000   0.00002   0.00000   0.00002   0.00000   0.00002   0.00000   0.00002   0.00000   0.00002   0.00000   0.00002   0.00000
N2                 0.00000   0.73317   0.04948   0.73323   0.04948   0.73329   0.04948   0.73334   0.04948   0.73339   0.04948   0.73341   0.04948
O                  0.00000   0.00006   0.00000   0.00005   0.00000   0.00004   0.00000   0.00003   0.00000   0.00002   0.00000   0.00001   0.00000
OH                 0.00000   0.00095   0.00000   0.00081   0.00000   0.00069   0.00000   0.00055   0.00000   0.00045   0.00000   0.00037   0.00000
O2                 0.00000   0.05145   0.00357   0.05147   0.00357   0.05150   0.00357   0.05152   0.00357   0.05155   0.00357   0.05156   0.00357
C6H6               0.00337   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315   0.00000   0.00315
C7H8               0.00604   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563   0.00000   0.00563
C8H18              0.00539   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502   0.00000   0.00502
AIR                0.98520   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887   0.00000   0.91887

TOTAL COMPUTER TIME=  14.713 SEC        DELTA TIME =  4.042 SEC
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STATIONS  5 - 6      CYCLE 4
EICHELBERG HEAT TRANSFER COEFICIENT


CRANKANGLE         0.0000   420.23   423.23   426.23   429.22   433.72   436.71   439.71   442.71   445.70   448.70   453.83
MASS,G             0.0000   0.5672   0.5673   0.5673   0.5673   0.5673   0.5673   0.5673   0.5673   0.5673   0.5673   0.5673
VOLUME,CC          0.0000   317.92   336.90   356.14   375.57   404.90   424.50   444.03   463.45   482.69   501.70   533.56
Q, CAL             0.0000   13.233   14.034   14.815   15.576   16.686   17.406   18.110   18.800   19.477   20.142   21.252
W, CAL             0.0000   44.300   48.410   52.276   55.910   60.952   64.055   66.966   69.694   72.251   74.644   78.395
FUMP W, CAL        0.0000   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761   9.3761
DELTA Q/DEL TH     0.0000   0.2708   0.2673   0.2606   0.2542   0.2469   0.2401   0.2351   0.2304   0.2259   0.2217   0.2164
DELTA W/DEL TH     0.0000   1.4132   1.3716   1.2904   1.2130   1.1217   1.0359   0.9715   0.9106   0.8531   0.7989   0.7306

P, ATM             0.5264   9.2895   8.6092   8.0013   7.4589   6.7508   6.3393   5.9697   5.6371   5.3373   5.0666   4.6613
T, DEG K            235.6   1840.5   1807.4   1775.8   1745.7   1703.4   1677.0   1651.9   1628.1   1605.6   1584.1   1550.0
RHO, G/CC        8.1081-4 1.7842-3 1.6838-3 1.5929-3 1.5105-3 1.4010-3 1.3364-3 1.2776-3 1.2240-3 1.1753-3 1.1307-3 1.0632-3
H, CAL/G          -54.284  -70.801  -81.680  -92.062  -101.87  -115.62  -124.17  -132.27  -139.93  -147.18  -154.04  -164.95
U, CAL/G          -70.006  -196.89  -205.50  -213.71  -221.46  -232.30  -239.05  -245.43  -251.46  -257.16  -262.56  -271.13
S, CAL/(G)(K)      1.5676   2.0213   2.0206   2.0198   2.0190   2.0179   2.0171   2.0164   2.0156   2.0149   2.0142   2.0129
CP, CAL/(G)(K)     0.2429   0.3259   0.3251   0.3243   0.3236   0.3225   0.3217   0.3210   0.3203   0.3197   0.3190   0.3180
GAMMA (S)          1.3787   1.2662   1.2670   1.2678   1.2686   1.2697   1.2705   1.2713   1.2720   1.2727   1.2734   1.2746
M, MOL WT          29.782   29.007   29.008   29.008   29.009   29.009   29.010   29.010   29.010   29.010   29.010   29.010

MOLE FRACTIONS

AR                0.00000  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883  0.00883
CO                0.00000  0.00005  0.00004  0.00003  0.00002  0.00002  0.00001  0.00001  0.00001  0.00001  0.00000  0.00000
CO2               0.00000  0.10312  0.10313  0.10314  0.10315  0.10316  0.10316  0.10317  0.10317  0.10317  0.10317  0.10317
H2                0.00000  0.00001  0.00001  0.00001  0.00001  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
H2O               0.00000  0.09731  0.09734  0.09737  0.09739  0.09742  0.09743  0.09745  0.09746  0.09746  0.09747  0.09748
NO                0.00000  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531  0.00531
NO2               0.00000  0.00002  0.00002  0.00002  0.00002  0.00002  0.00002  0.00002  0.00002  0.00002  0.00002  0.00003
N2                0.00000  0.73341  0.73343  0.73344  0.73346  0.73347  0.73348  0.73348  0.73349  0.73349  0.73349  0.73350
O                 0.00000  0.00001  0.00001  0.00001  0.00001  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
OH                0.00000  0.00037  0.00031  0.00026  0.00022  0.00017  0.00015  0.00013  0.00011  0.00009  0.00008  0.00007
O2                0.00000  0.05156  0.05157  0.05158  0.05159  0.05160  0.05160  0.05160  0.05161  0.05161  0.05161  0.05162
C6H6              0.00337  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
C7H8              0.00604  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
C8H18             0.00539  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
AIR               0.98520  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   4    LEVEL 1    CASE NO.      512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =    8.5      RPM = 2140.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                          WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                               CAL/MOL           DEC K
FUEL     C  8.00000   H 18.00000                                             0.428571  -59820.961  L      298.15
FUEL     C  7.00000   H  8.00000                                             0.387755    2867.033  L      298.15
FUEL     C  6.00000   H  6.00000                                             0.183673   11718.145  L      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  *1.000000   -1047.375  G      298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER          RELATIVE HUMIDITY= 0.5500

                 A/F= 19.7493   PERCENT FUEL=   4.8194   EQUIVALENCE RATIO= 0.7367   PHI=   0.7250
FUEL MASS FRACTION = 0.045805                           INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  5.7966
AIR MASS FRACTION = 0.904610                            PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.4421
RESIDUAL MASS FRACTION = 0.049585                       CHEMICAL ENERGY (JOULES/G) =2052.251
RECIRCULATED MASS FRACTION = 0.000000                   MASS EFFICIENCY = 0.950415
MASS FRACTION EXHAUST RETAINED = 0.049557               VOLUME EFFICIENCY = 0.809222
NET WORK EFFICIENCY = 0.343192                          FRACTIONAL MASS CHANGE 6 - 7 =-0.578769

THERMODYNAMIC PROPERTIES

STATION                         2        3        4        5        6        7
CRANKANGLE       0.0000   29.376   180.00   332.00   332.00   540.00   540.00   0.0000
P, ATM           0.5264   0.5264   0.5264   5.2554   24.950   2.9799   0.9840   0.9840
T, DEG K          235.6   1053.5    280.7    516.3   2386.0   1550.0   1215.1    298.1
RHO, G/CC      8.1081-4 1.7665-4 6.7966-4 3.6897-3 3.6897-3 6.7966-4 2.8630-4 1.2521-3
H, CAL/G        -54.284  -315.07  -67.215  -7.5770   121.69  -162.04  -266.54  -553.43
U, CAL/G        -70.006  -387.23  -85.971  -42.071  -42.071  -268.21  -349.78  -572.46
S, CAL/(G)(K)    1.5676   2.0447   1.6278   1.6278   2.0448   2.0448   2.0448   1.5799
CP, CAL/(G)(K)   0.2429   0.2976   0.2453   0.2622   0.3933   0.3188   0.3054   0.9295
GAMMA (S)        1.3787   1.2990   1.3743   1.3419   1.2222   1.2738   1.2892   1.1609
M, MOL WT        29.782   29.010   29.742   29.742   28.953   29.010   29.010   31.130

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR              0.00000  0.00883  0.00045  0.00045  0.00881  0.00883  0.00883  0.00883
CO              0.00000  0.00000  0.00000  0.00000  0.00176  0.00000  0.00000  0.00000
CO2             0.00000  0.10312  0.00524  0.00524  0.10121  0.10317  0.10317  0.10318
H               0.00000  0.00000  0.00000  0.00000  0.00005  0.00000  0.00000  0.00000
HO2             0.00000  0.00000  0.00000  0.00000  0.00001  0.00000  0.00000  0.00000
H2              0.00000  0.00000  0.00000  0.00000  0.00029  0.00000  0.00000  0.00000
H2O(L)          0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.06809
H2O             0.00000  0.09744  0.00495  0.00495  0.09546  0.09748  0.09748  0.02942
NO              0.00000  0.00918  0.00047  0.00047  0.00917  0.00919  0.00919  0.00000
NO2             0.00000  0.00000  0.00000  0.00000  0.00002  0.00000  0.00000  0.00000
N2              0.00000  0.73158  0.03719  0.03719  0.73011  0.73156  0.73156  0.73617
O               0.00000  0.00000  0.00000  0.00000  0.00036  0.00000  0.00000  0.00000
OH              0.00000  0.00006  0.00000  0.00000  0.00309  0.00006  0.00006  0.0000
O2              0.00000  0.04977  0.00253  0.00253  0.04967  0.04970  0.04970  0.05431
C6H6            0.00337  0.00000  0.00320  0.00320  0.00000  0.00000  0.00000  0.00000
C7H8            0.00604  0.00000  0.00573  0.00573  0.00000  0.00000  0.00000  0.00000
C8H18           0.00539  0.00000  0.00511  0.00511  0.00000  0.00000  0.00000  0.00000
AIR             0.98520  0.00000  0.93512  0.93512  0.00000  0.00000  0.00000  0.00000
TOTAL COMPUTER TIME=   0.723 SEC        DELTA TIME =  0.123 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   1    LEVEL 2    CASE NO.      512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =   8.5     RPM = 2140.0     EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.160 CM     STROKE =  8.839 CM     ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME =  812.15 CC     DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.44 DEG     IVSHUT = 180.00 DEG                             EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =   0.500000  -0.500000

                                                                            WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL           DEG K
FUEL    C  8.00000    H 18.00000                                               0.428571  -59820.961  L     298.15
FUEL    C  7.00000    H  8.00000                                               0.387755    2867.033  L     298.15
FUEL    C  6.00000    H  6.00000                                               0.183673   11718.145  L     298.15
AIR     N  1.56168    O  0.41959   AR 0.00936   C  0.00032                    *1.000000   -1047.375  G     298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER             RELATIVE HUMIDITY= 0.5500

                    A/F= 19.7493   PERCENT FUEL=   4.8194   EQUIVALENCE RATIO= 0.7367    PHI=    0.7250

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.55688                   CHARGE        9.4431                    EXHAUST        9.2735
     FUEL           0.02552                   FUEL          0.4551                    CO            0.00000
     AIR            0.50400                   AIR           8.9880                    NOX           0.02628

   ENERGY PER CYCLE (JOULES)             AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK         424.650          INDICATED POWER           7.573            NET WORK        0.343181
 INDICATED PUMP WORK    -32.267          INDICATED PUMP POWER     -0.575            HEAT LOSS       0.164728
 HEAT LOSS              188.346          HEAT LOSS RATE            3.359            EXHAUST         0.439578
 CHEM. ENERGY          1143.372          EXHAUST POWER             8.963

                                                      MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)               5.8484
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -0.4444
                               MEAN TORQUE (NEWTON-METERS)                          31.2248

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1009.46 K  AND  0.9840 ATM     MOLECULAR WEIGHT =  29.011
     AR        0.008829      CO2        0.103178      H2O       0.097511      NO        0.002737      N2        0.734798
     OH        0.000005      O2         0.052939

FRESH CHARGE MOLE FRACTIONS AT  235.63 K  AND  0.5264 ATM      MOLECULAR WEIGHT =  29.782
     C6H6      0.003375      C7H8       0.006040      C8H18     0.005385      AIR       0.985199

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   2.978 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                        CYCLE   2    LEVEL 2    CASE NO.      512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =   8.5      RPM = 2140.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.160 CM     STROKE =  8.839 CM     ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM      WALL TEMP =   360.0 K
TOTAL VOLUME =  812.15 CC      DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.94 DEG     IVSHUT = 180.00 DEG                              EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000


         AN =    0.500000  -0.500000

                                                                         WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                               CAL/MOL           DEG K
FUEL    C  8.00000   H 18.00000                                            0.428571    -59820.961  L      298.15
FUEL    C  7.00000   H  8.00000                                            0.387755      2867.033  L      298.15
FUEL    C  6.00000   H  6.00000                                            0.183673     11718.145  L      298.15
AIR     N  1.56168   O  0.41959    AR 0.00936    C  0.00032               *1.000000     -1047.375  G      298.15
                  * AIR INCLUDES    0.01762 MOLE FRACTION WATER          RELATIVE HUMIDITY= 0.5500
                  A/F= 19.7493   PERCENT FUEL=   4.8194   EQUIVALENCE RATIO= 0.7367   PHI=    0.7250
                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.56686                   CHARGE       9.4516                     EXHAUST        9.4446
     FUEL          0.02554                   FUEL         0.4555                     CO             0.00000
     AIR           0.50445                   AIR          8.9960                     NOX            0.02471

   ENERGY PER CYCLE (JOULES)             AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK           426.735       INDICATED POWER          7.610              NET WORK        0.344586
 INDICATED PUMP WORK      -32.220       INDICATED PUMP POWER    -0.575              HEAT LOSS       0.159707
 HEAT LOSS                182.848       HEAT LOSS RATE           3.261              EXHAUST         0.438529
 CHEM. ENERGY            1144.896       EXHAUST POWER            8.954
                                                 MISCELLANEOUS

                           INDICATED MEAN EFFECTIVE PRESSURE (ATM)            5.8771
                           PUMP MEAN EFFECTIVE PRESSURE (ATM)                -0.4437
                           MEAN TORQUE (NEWTON-METERS)                       31.3945

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  996.56 K  AND  0.9840 ATM      MOLECULAR WEIGHT =  29.011
     AR        0.008829       CO2       0.103178       H2O       0.097512       NO        0.002527       N2         0.734903
     O2        0.053044

FRESH CHARGE MOLE FRACTIONS AT  235.63 K  AND  0.5264 ATM      MOLECULAR WEIGHT =  29.782
     C6H6      0.003375       C7H8      0.006040       C8H18     0.005385       AIR       0.985199

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   3.088 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   3    LEVEL 2     CASE NO.      512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =   8.5     RPM = 2140.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.160 CM     STROKE =  8.839 CM     ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME =  812.15 CC     DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.95 DEG     IVSHUT = 180.00 DEG                         EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =   0.500000  -0.500000

                                                                            WT FRACTION   ENERGY    STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL           DEG K
FUEL    C  8.00000   H 18.00000                                                0.428571   -59820.961   L    298.15
FUEL    C  7.00000   H  8.00000                                                0.387755     2867.033   L    298.15
FUEL    C  6.00000   H  6.00000                                                0.183673    11718.145   L    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                     *1.000000    -1047.375   G    298.15
                 * AIR INCLUDES   0.01762 MOLE FRACTION WATER              RELATIVE HUMIDITY= 0.5500

                  A/F= 19.7493   PERCENT FUEL=   4.8194   EQUIVALENCE RATIO= 0.7367   PHI=    0.7250

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL       0.56727                       CHARGE       9.4520                        EXHAUST       9.4517
     FUEL        0.02554                       FUEL         0.4555                        CO           0.00000
     AIR         0.50447                       AIR          8.9965                        NOX          0.02465

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK        426.823             INDICATED POWER         7.612                NET WORK       0.344643
 INDICATED PUMP WORK   -32.219             INDICATED PUMP POWER   -0.575                HEAT LOSS      0.159514
 HEAT LOSS             182.638             HEAT LOSS RATE          3.257                EXHAUST        0.438485
 CHEM. ENERGY         1144.967             EXHAUST POWER           8.953

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)             5.8783
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.4437
                              MEAN TORQUE (NEWTON-METERS)                        31.4016

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  996.04 K  AND  0.9840 ATM      MOLECULAR WEIGHT =  29.011
     AR       0.008829      CO2      0.103178      H2O      0.097512      NO       0.002519      N2        0.734908
     O2       0.053048

FRESH CHARGE MOLE FRACTIONS AT  235.63 K  AND  0.5264 ATM      MOLECULAR WEIGHT =  29.782
     C6H6     0.003375      C7H8     0.006040      C8H18    0.005385      AIR      0.985199

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   3.062 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  8    LEVEL 3    CASE NO.     512
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =   8.5     RPM = 2140.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.160 CM     STROKE =  8.839 CM     ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME =  812.15 CC     DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.95 DEG     IVSHUT = 180.00 DEG                          EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME     FINITE BURNING INTERVAL = 88.2 DEG     COSINE  COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =   0.500000  -0.500000
                                                                          WT FRACTION    ENERGY    STATE     TEMP
         CHEMICAL FORMULA                                                                CAL/MOL              DEG K
FUEL     C  8.00000   H 18.00000                                              0.428571    -59820.961  L      298.15
FUEL     C  7.00000   H  8.00000                                              0.387755      2867.033  L      298.15
FUEL     C  6.00000   H  6.00000                                              0.183673     11718.145  L      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936    C  0.00032                  *1.000000     -1047.375  G      298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER          RELATIVE HUMIDITY= 0.5500

                     A/F= 19.7493    PERCENT FUEL=    4.8194   EQUIVALENCE RATIO= 0.7367    PHI=    0.7250

                                            PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                    MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.56738                      CHARGE          9.4521                       EXHAUST        9.4522
     FUEL           0.02554                      FUEL            0.4555                       CO             0.00000
     AIR            0.50448                      AIR             8.9966                       NOX            0.05233

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK         425.749             INDICATED POWER          7.593              NET WORK       0.343599
 INDICATED PUMP WORK    -32.218             INDICATED PUMP POWER    -0.575              HEAT LOSS      0.158376
 HEAT LOSS              181.391             HEAT LOSS RATE           3.235              EXHAUST        0.440792
 CHEM. ENERGY          1145.319             EXHAUST POWER            9.003

                                                       MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              5.8635
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.4437
                              MEAN TORQUE (NEWTON-METERS)                         31.3162

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  993.39 K  AND  0.9840 ATM      MOLECULAR WEIGHT =  29.011
     AR        0.008829        CO2        0.103179       H2O        0.097513       NO         0.005298        NO2        0.000035
     N2        0.733512        OH         0.000006       O2         0.051626

FRESH CHARGE MOLE FRACTIONS AT  235.63 K  AND  0.5264 ATM      MOLECULAR WEIGHT =  29.782
     C6H6      0.003375        C7H8       0.006040       C8H18      0.005385       AIR        0.985199

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   5.661 SEC
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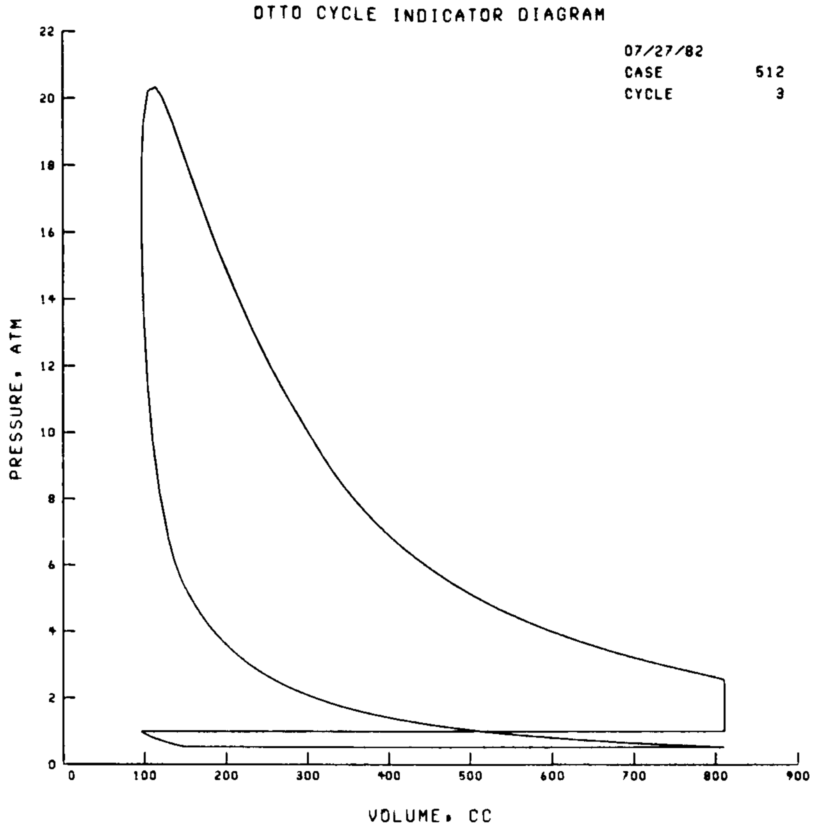
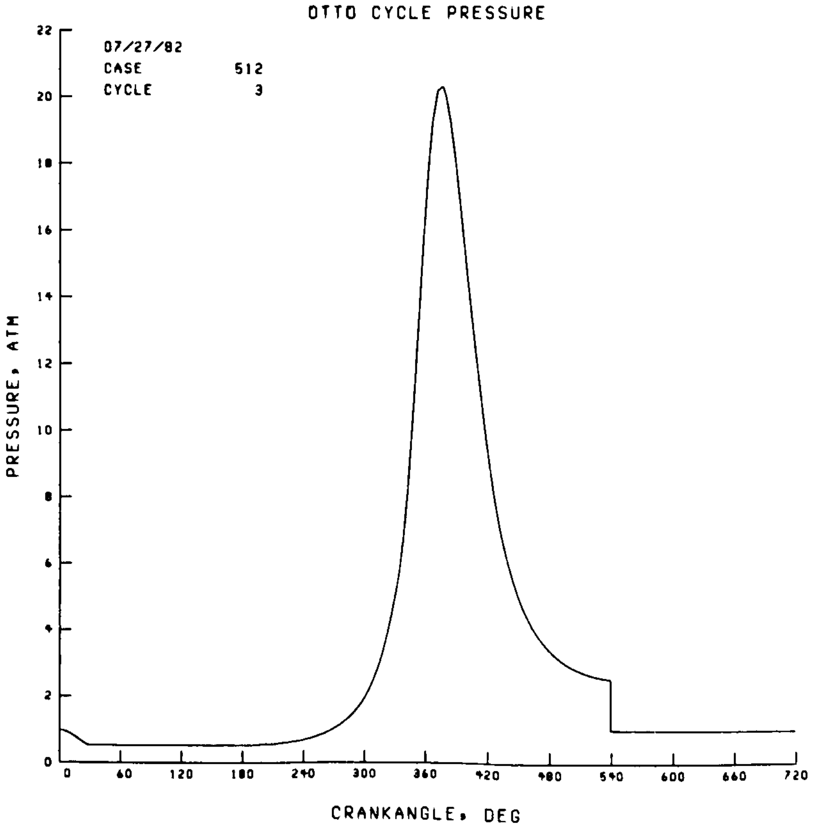
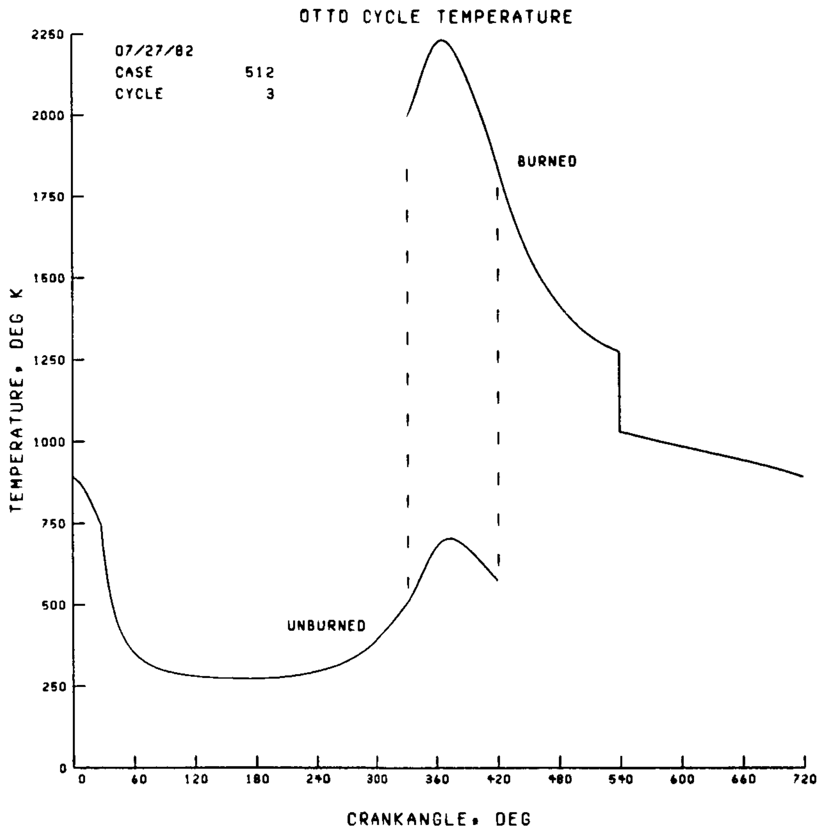
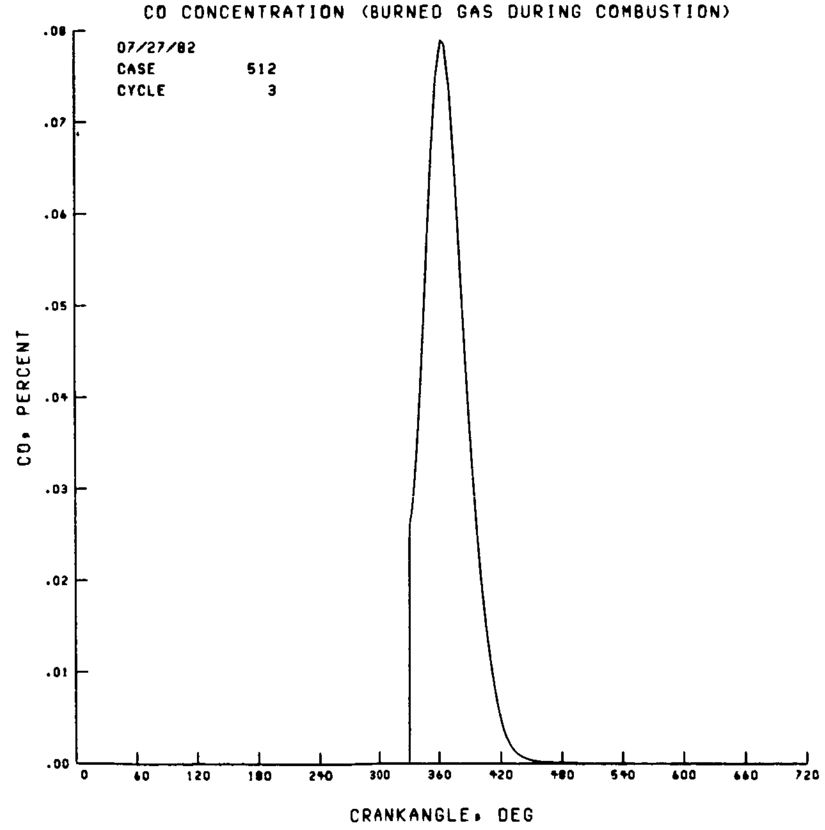

OTTO CYCLE INDICATOR DIAGRAM

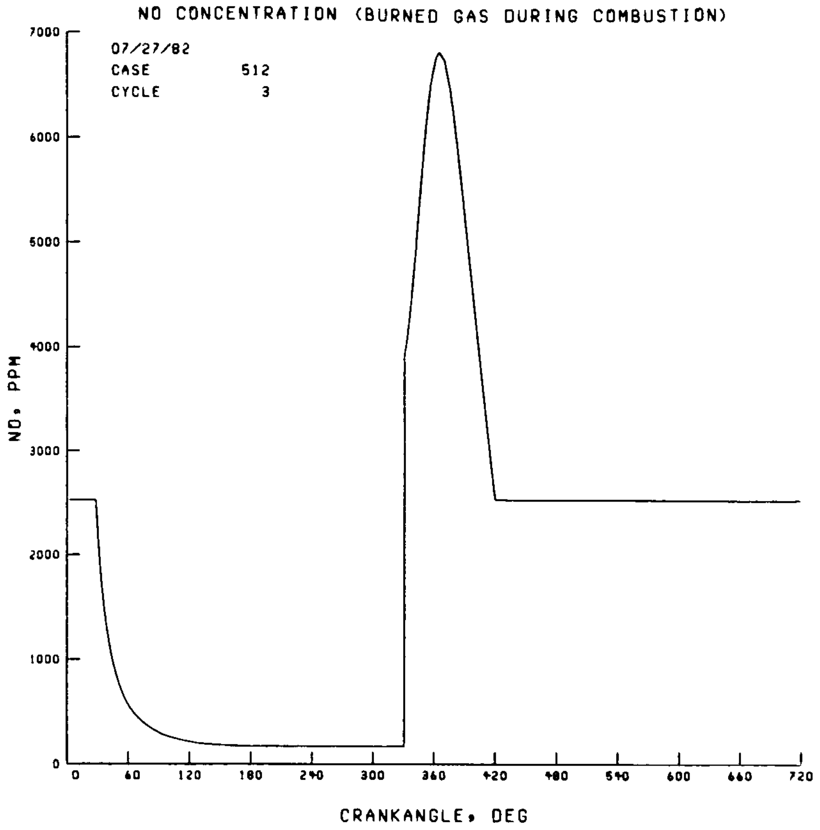

OTTO CYCLE PRESSURE

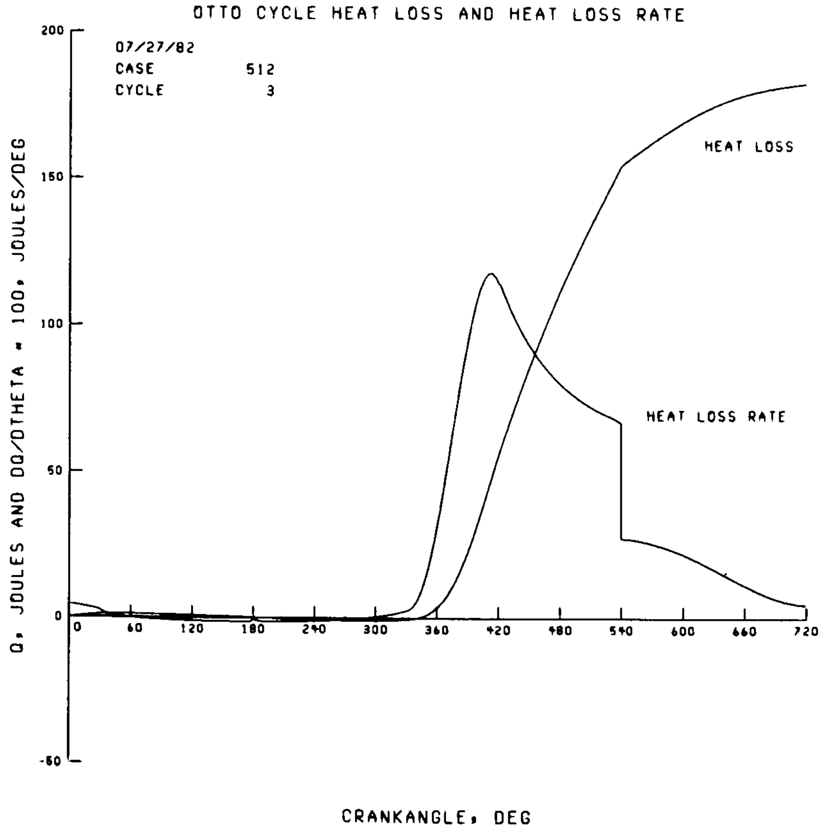


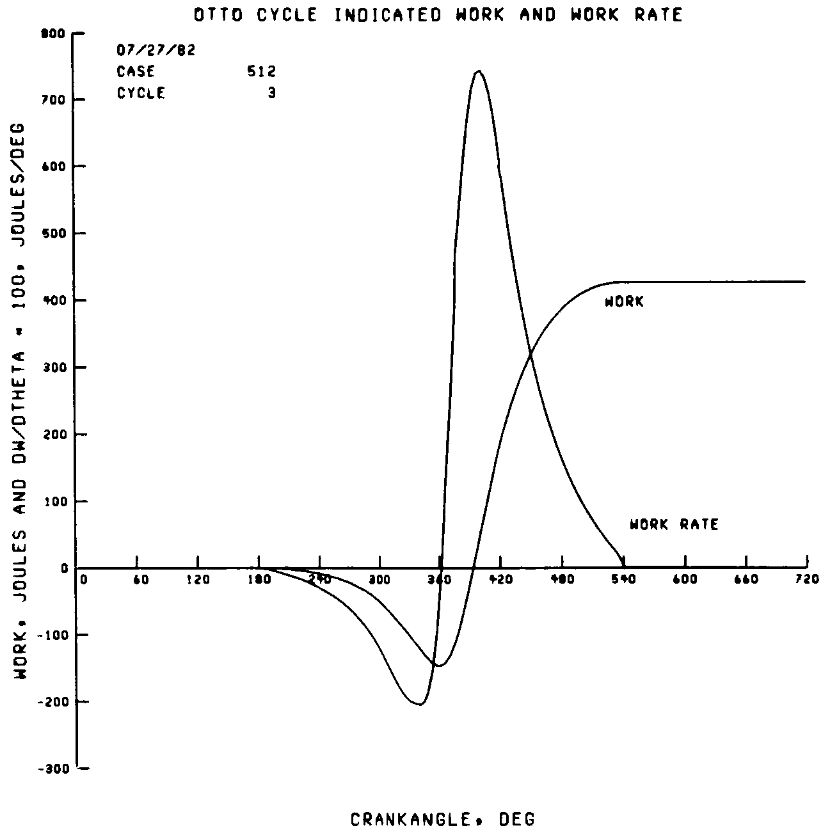
OTTO CYCLE TEMPERATURE

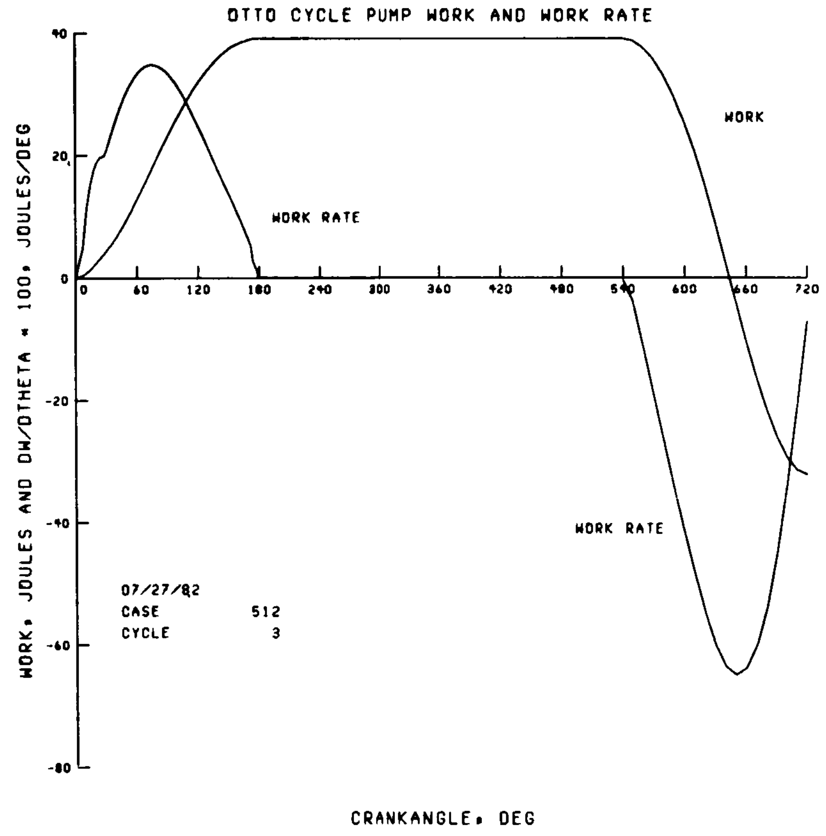


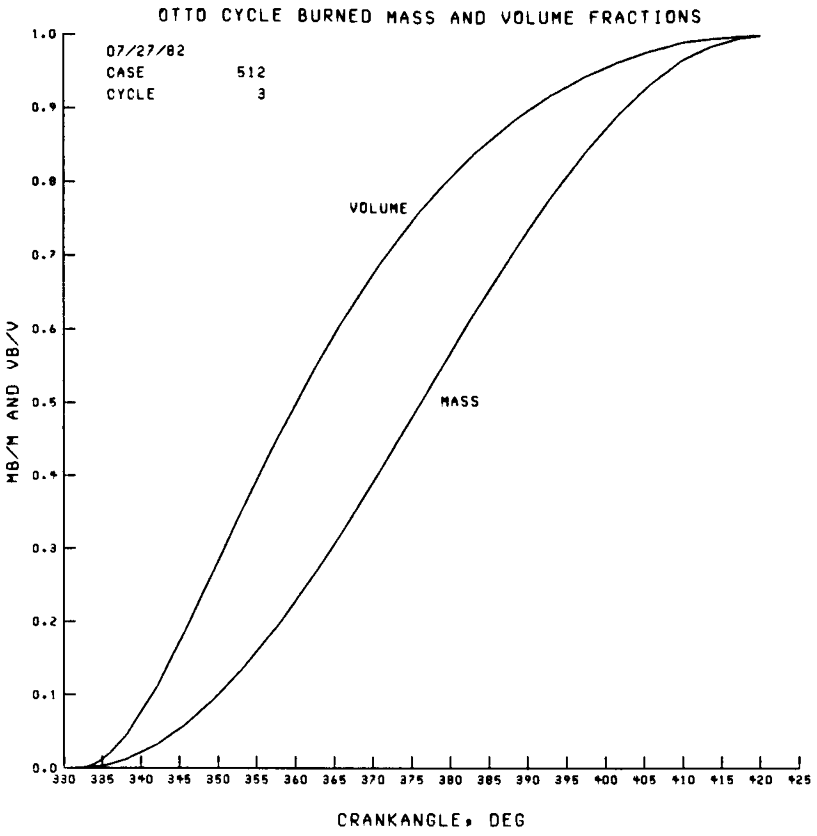
CO CONCENTRATION (BURNED GAS DURING COMBUSTION)

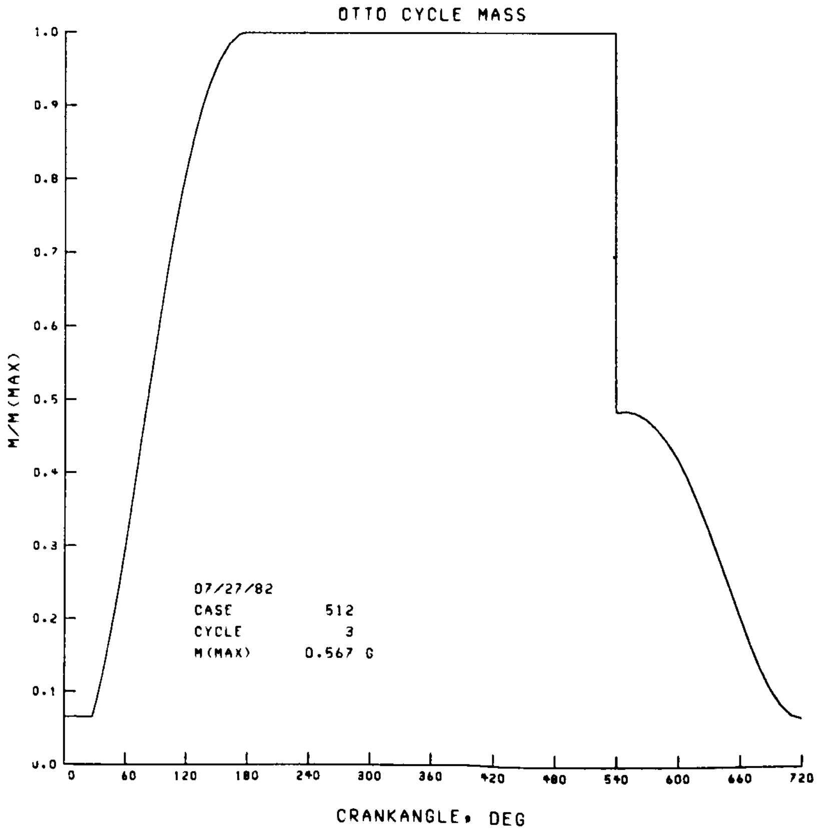

NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 512
CYCLE 3
NO, PPM
7000
6000
5000
4000
3000
2000
1000
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

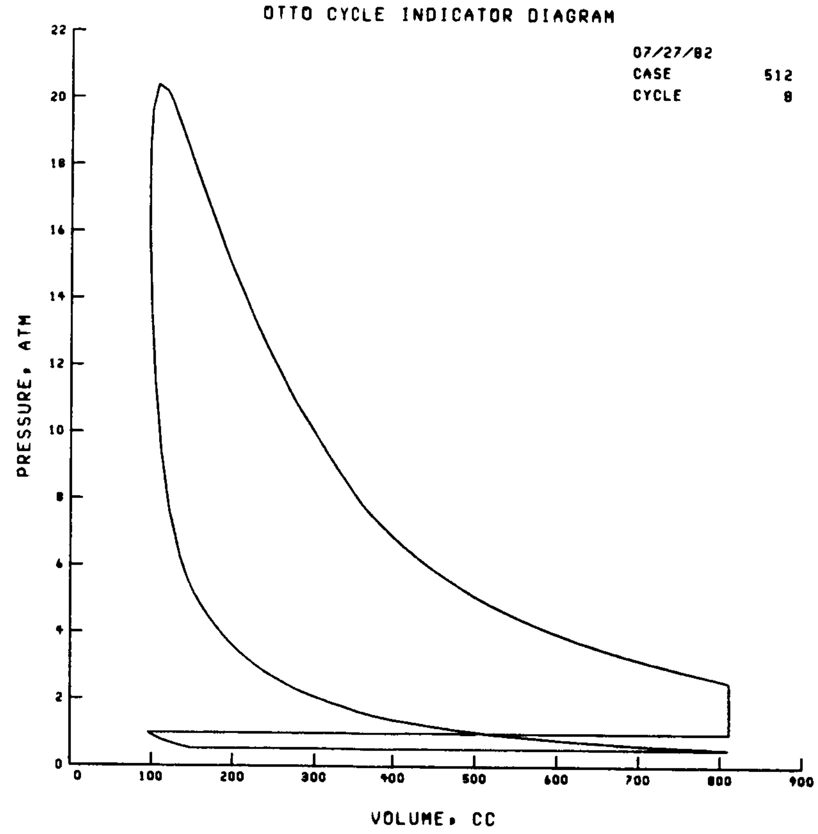

OTTO CYCLE HEAT LOSS AND HEAT LOSS RATE
07/27/82
CASE 512
CYCLE 3
HEAT LOSS
HEAT LOSS RATE
Q, JOULES AND DQ/DTHETA * 100, JOULES/DEG
200
150
100
50
0
-50
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

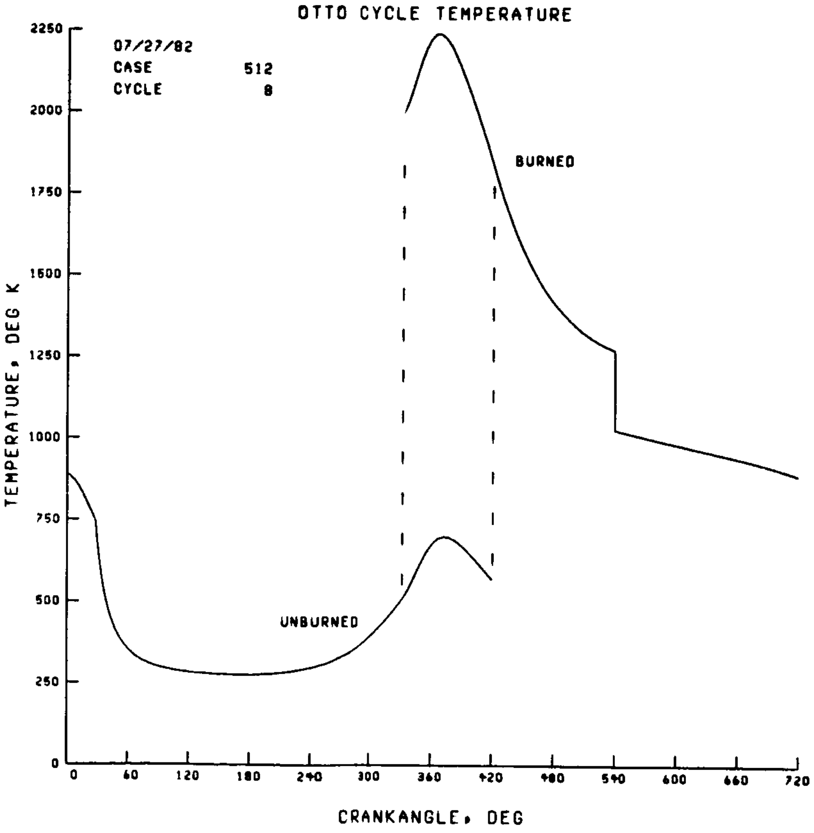

OTTO CYCLE INDICATED WORK AND WORK RATE
07/27/82
CASE 512
CYCLE 3
WORK
WORK RATE
WORK, JOULES AND DW/DTHETA * 100, JOULES/DEG
800
700
600
500
400
300
200
100
0
-100
-200
-300
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

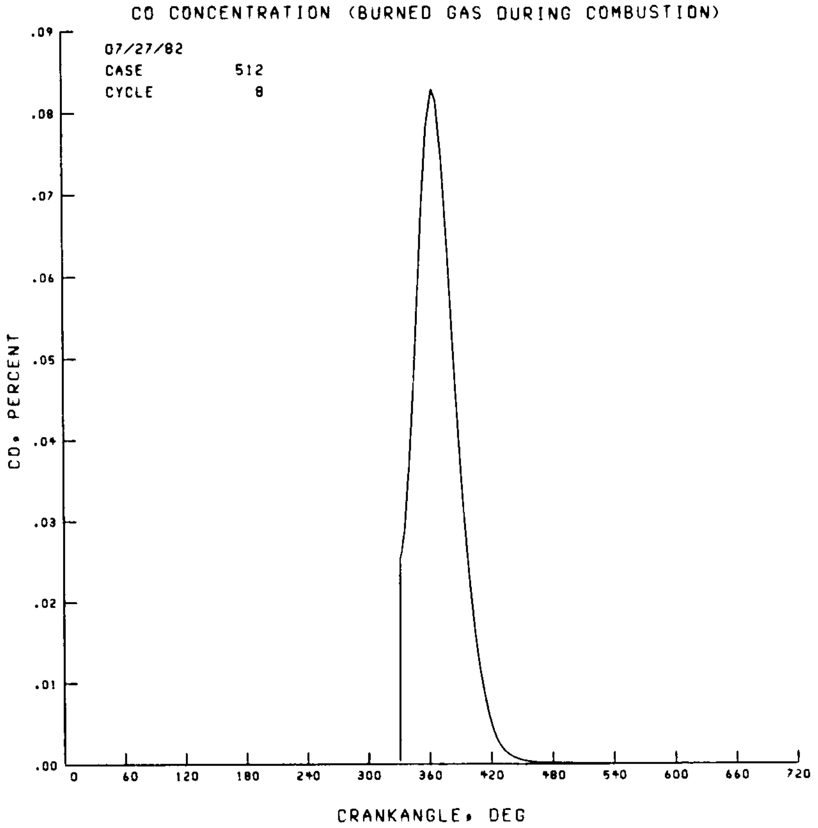

OTTO CYCLE PUMP WORK AND WORK RATE
WORK
WORK RATE
WORK RATE
07/27/82
CASE 512
CYCLE 3
WORK, JOULES AND DW/DTHETA * 100, JOULES/DEG
40
20
0
-20
-40
-60
-80
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

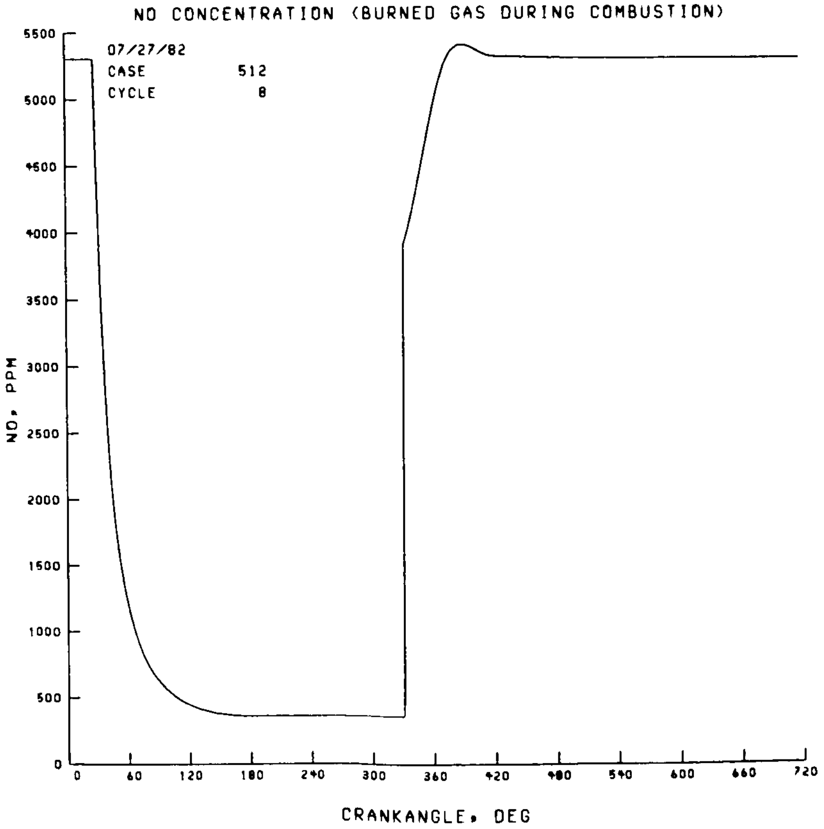

OTTO CYCLE BURNED MASS AND VOLUME FRACTIONS
07/27/82
CASE 512
CYCLE 3
VOLUME
MASS
MB/M AND VB/V
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
330
335
340
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
425
CRANKANGLE, DEG


OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
07/27/82
CASE 512
CYCLE 3
M(MAX) 0.567 G
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


OTTO CYCLE INDICATOR DIAGRAM
07/27/82
CASE 512
CYCLE 8
PRESSURE, ATM
0
2
4
6
8
10
12
14
16
18
20
22
0
100
200
300
400
500
600
700
800
900
VOLUME, CC


OTTO CYCLE TEMPERATURE
07/27/82
CASE 512
CYCLE 8
BURNED
UNBURNED
TEMPERATURE, DEG K
0
250
500
750
1000
1250
1500
1750
2000
2250
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 512
CYCLE 8
CO, PERCENT
.09
.08
.07
.06
.05
.04
.03
.02
.01
.00
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 512
CYCLE 8
NO, PPM
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

Input, Case 513

```
REAC
C 8.      H 18.                                   .42               L298.15  F
C 7.      H 8.                                    .38               L298.15  F
C 6.      H 6.                                    .18               L298.15  F

NAME
 &OTTINP FREQ=2140,BORE=10.16,STROKE=8.839,ROD=14.478,CA=80.,
 TW=360.,CR= 8.5,CSBURN=T,KASE=513,
 PEXH=.9840,PMFOLD=.5264,
   HC3=0.,HA=.0,HB=.0,HC2=.0000,
   HP=T,RHUMID=55.,TAIR=298.15&END
 &AFINP PHI=.725,SPARK=28.0,EGR=0.,THBURN=88.8,
   NCYCLE=8,KINET=4,TAU=0.00E-00,DEBUG=T,VARAF=F&END
```

Output, Case 513

Cycle Summary Sheets

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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                   CYCLE   4    LEVEL 1    CASE NO.      513
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =    8.5     RPM = 2140.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM     MANIFOLD PRESSURE = 0.52640 ATM      EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES MINIMIZE INTERNAL ENERGY CHANGES

                                                                         WT FRACTION    ENERGY   STATE     TEMP
            CHEMICAL FORMULA                                                            CAL/MOL            DEG K
FUEL     C  8.00000   H 18.00000                                           0.428571   -59820.961  L       298.15
FUEL     C  7.00000   H  8.00000                                           0.387755     2867.033  L       298.15
FUEL     C  6.00000   H  6.00000                                           0.183673    11718.145  L       298.15
AIR      N  1.56168   O  0.41959    AR 0.00936    C  0.00032              *1.000000    -1047.375  G       298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER         RELATIVE HUMIDITY= 0.5500

                   A/F= 19.7493    PERCENT FUEL=    4.8194   EQUIVALENCE RATIO= 0.7367    PHI=   0.7250
FUEL MASS FRACTION = 0.045934                          INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  5.5614
AIR MASS FRACTION = 0.907173                           PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.4420
RESIDUAL MASS FRACTION = 0.046893                      CHEMICAL ENERGY (JOULES/G) =2057.733
RECIRCULATED MASS FRACTION = 0.000000                  MASS EFFICIENCY = 0.953107
MASS FRACTION EXHAUST RETAINED = 0.046873              VOLUME EFFICIENCY = 0.808752
NET WORK EFFICIENCY = 0.341046                         FRACTIONAL MASS CHANGE 6 - 7 =-0.601583

THERMODYNAMIC PROPERTIES

STATION                          2         3         4         5         6         7
CRANKANGLE         0.0000    29.480    180.00    332.00    332.00    540.00    540.00    0.0000
P, ATM             0.5264    0.5264    0.5264    5.2360    24.102    2.8833    0.9840    0.9840
T, DEG K            244.1    1163.8     292.6     536.1    2401.6    1563.0    1338.9     298.1
RHO, G/CC       7.8277-4 1.5991-4 6.5217-4 3.5404-3 3.5404-3 6.5217-4 2.5983-4 1.2521-3
H, CAL/G          -52.231   -281.74   -62.994   -1.0580    127.99   -157.69   -228.22   -553.43
U, CAL/G          -68.517   -361.46   -82.541   -36.873   -36.873   -264.76   -319.93   -572.47
S, CAL/(G)(K)      1.5762    2.0747    1.6372    1.6372    2.0498    2.0498    2.0748    1.5799
CP, CAL/(G)(K)     0.2433    0.3030    0.2459    0.2639    0.3974    0.3193    0.3105    0.9295
GAMMA (S)          1.3779    1.2921    1.3730    1.3390    1.2205    1.2733    1.2830    1.1609
M, MOL WT          29.782    29.010    29.745    29.745    28.947    29.010    29.010    31.130

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR                0.00000  0.00883  0.00042  0.00042  0.00881  0.00883  0.00883  0.00883
CO                0.00000  0.00000  0.00000  0.00000  0.00195  0.00000  0.00000  0.00000
CO2               0.00000  0.10313  0.00496  0.00496  0.10100  0.10317  0.10317  0.10318
H                 0.00000  0.00000  0.00000  0.00000  0.00006  0.00000  0.00000  0.00000
HO2               0.00000  0.00000  0.00000  0.00000  0.00001  0.00000  0.00000  0.00000
H2                0.00000  0.00000  0.00000  0.00000  0.00031  0.00000  0.00000  0.00000
H2O(L)            0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.06809
H2O               0.00000  0.09744  0.00468  0.00468  0.09531  0.09747  0.09747  0.02942
NO                0.00000  0.00945  0.00045  0.00045  0.00943  0.00945  0.00945  0.00000
NO2               0.00000  0.00000  0.00000  0.00000  0.00002  0.00000  0.00000  0.00000
N2                0.00000  0.73144  0.03517  0.03517  0.72984  0.73143  0.73143  0.73617
O                 0.00000  0.00000  0.00000  0.00000  0.00039  0.00000  0.00000  0.00000
OH                0.00000  0.00007  0.00000  0.00000  0.00328  0.00007  0.00007  0.00000
O2                0.00000  0.04963  0.00239  0.00239  0.04958  0.04957  0.04957  0.05431
C6H6              0.00337  0.00000  0.00321  0.00321  0.00000  0.00000  0.00000  0.00000
C7H8              0.00604  0.00000  0.00575  0.00575  0.00000  0.00000  0.00000  0.00000
C8H18             0.00539  0.00000  0.00513  0.00513  0.00000  0.00000  0.00000  0.00000
AIR               0.98520  0.00000  0.93783  0.93783  0.00000  0.00000  0.00000  0.00000

TOTAL COMPUTER TIME=   0.723 SEC        DELTA TIME =  0.127 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   3    LEVEL 2    CASE NO.      513
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =   8.5      RPM = 2140.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM      MANIFOLD PRESSURE = 0.52640 ATM      EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES MINIMIZE INTERNAL ENERGY CHANGES
BORE = 10.160 CM      STROKE =  8.839 CM      ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME =  812.15 CC      DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.89 DEG      IVSHUT = 180.00 DEG                                EVOPEN = 540.00 DEG      EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME     FINITE BURNING INTERVAL = 88.2 DEG     COSINE  COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.500000  -0.500000
                                                                           WT FRACTION    ENERGY    STATE    TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL            DEG K
FUEL     C  8.00000    H 18.00000                                             0.428571    -59820.961  L      298.15
FUEL     C  7.00000    H  8.00000                                             0.387755      2867.033  L      298.15
FUEL     C  6.00000    H  6.00000                                             0.183673     11718.145  L      298.15
AIR      N  1.56168    O  0.41959    AR 0.00936    C  0.00032                *1.000000     -1047.375  G      298.15
                     * AIR INCLUDES    0.01762 MOLE FRACTION WATER          RELATIVE HUMIDITY= 0.5500

                     A/F= 19.7493    PERCENT FUEL=    4.8194    EQUIVALENCE RATIO= 0.7367    PHI=    0.7250
                                            PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                    MEAN INLET MASS FLOW RATE (G/SEC)          MEAN EXHAUST MASS FLOW RATE (G/SEC)

         TOTAL          0.54762                  CHARGE         9.1360                       EXHAUST         9.1358
         FUEL           0.02469                  FUEL           0.4403                       CO              0.00000
         AIR            0.48761                  AIR            8.6957                       NOX             0.02449

     ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

   INDICATED WORK          410.812          INDICATED POWER            7.326             NET WORK       0.342110
   INDICATED PUMP WORK     -32.225          INDICATED PUMP POWER      -0.575             HEAT LOSS      0.168364
   HEAT LOSS               186.315          HEAT LOSS RATE             3.323             EXHAUST        0.482787
   CHEM. ENERGY           1106.624          EXHAUST POWER              9.528
                                                         MISCELLANEOUS

                             INDICATED MEAN EFFECTIVE PRESSURE (ATM)              5.6578
                             PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.4438
                             MEAN TORQUE (NEWTON-METERS)                         30.1270

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1066.72 K   AND  0.9840 ATM       MOLECULAR WEIGHT =  29.011
    AR         0.008829       CO2        0.103178       H2O        0.097512       NO         0.002589       N2         0.734872
    O2         0.053013

FRESH CHARGE MOLE FRACTIONS AT  244.07 K  AND  0.5264 ATM       MOLECULAR WEIGHT =  29.782
    C6H6       0.003375       C7H8       0.006040       C8H18      0.005385       AIR        0.985199

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   3.101 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                            CYCLE   8    LEVEL 3    CASE NO.      513
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1982.

COMPRESSION RATIO =    8.5     RPM = 2140.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =  28.00 DEG
FUEL PRESSURE = 0.98400 ATM      MANIFOLD PRESSURE = 0.52640 ATM     EXHAUST PRESSURE = 0.98400 ATM
PRESSURE DISCONTINUITIES MINIMIZE INTERNAL ENERGY CHANGES
BORE = 10.160 CM      STROKE =  8.839 CM      ROD = 14.478 CM     CHAMBER AREA = 80.000 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME =  812.15 CC     DISPLACEMENT VOLUME =  716.61 CC

IVOPEN =  27.89 DEG      IVSHUT = 180.00 DEG                            EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME     FINITE BURNING INTERVAL = 88.2 DEG    COSINE  COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =    0.500000  -0.500000

                                                                                  WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                        CAL/MOL           DEG K
FUEL     C  8.00000   H 18.00000                                                     0.428571    -59820.961  L     298.15
FUEL     C  7.00000   H  8.00000                                                     0.387755      2867.033  L     298.15
FUEL     C  6.00000   H  6.00000                                                     0.183673     11718.145  L     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                          *1.000000     -1047.375  G     298.15
                    * AIR INCLUDES   0.01762 MOLE FRACTION WATER                 RELATIVE HUMIDITY= 0.5500

                  A/F= 19.7493    PERCENT FUEL=    4.8194   EQUIVALENCE RATIO= 0.7367    PHI=    0.7250


                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                         MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.54772                            CHARGE         9.1361                      EXHAUST        9.1360
     FUEL           0.02469                            FUEL           0.4403                      CO             0.00000
     AIR            0.48761                            AIR            8.6958                      NOX            0.05223

   ENERGY PER CYCLE (JOULES)                     AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK          409.712                 INDICATED POWER          7.307                NET WORK       0.341013
 INDICATED PUMP WORK     -32.225                 INDICATED PUMP POWER    -0.575                HEAT LOSS      0.167056
 HEAT LOSS               184.924                 HEAT LOSS RATE           3.298                EXHAUST        0.484651
 CHEM. ENERGY           1106.960                 EXHAUST POWER            9.567
                                                              MISCELLANEOUS

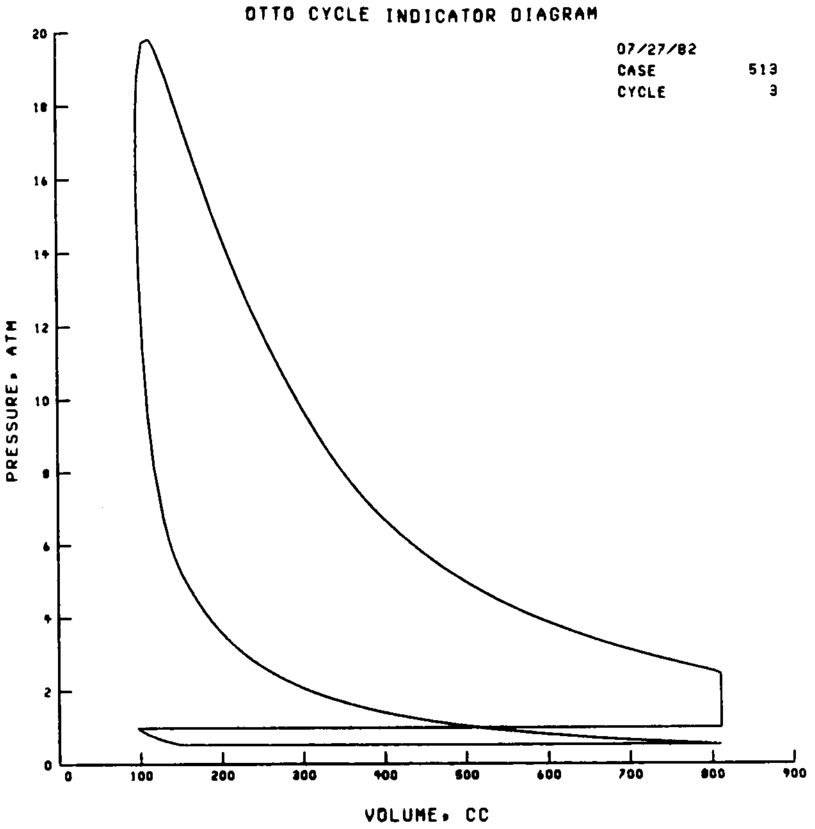
                                       INDICATED MEAN EFFECTIVE PRESSURE (ATM)              5.6426
                                       PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.4438
                                       MEAN TORQUE (NEWTON-METERS)                         30.0395

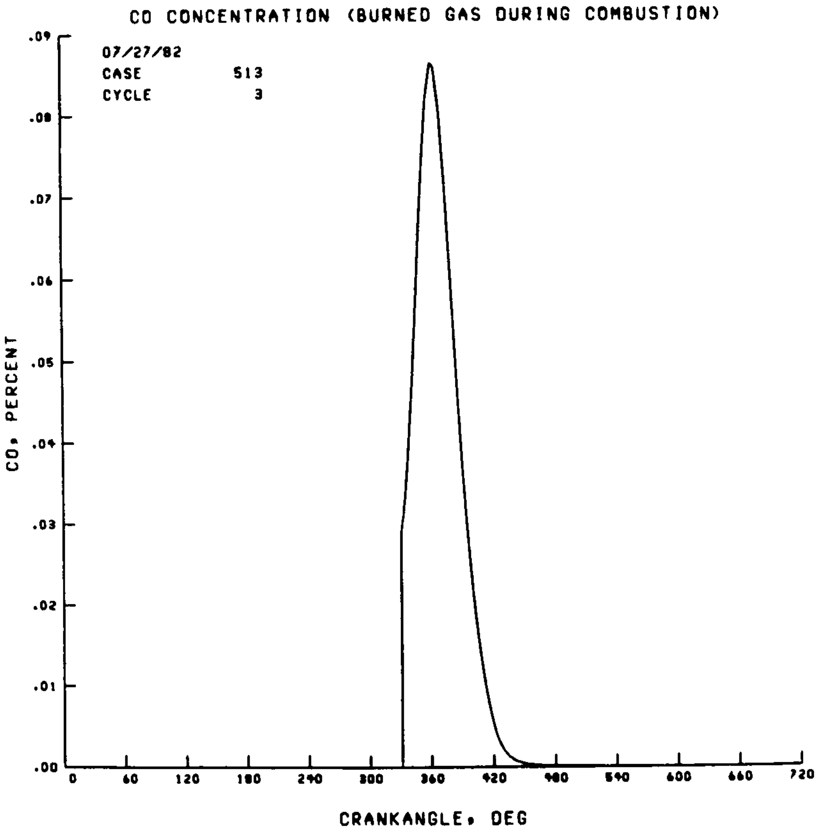
COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1063.19 K  AND  0.9840 ATM      MOLECULAR WEIGHT =  29.011
     AR        0.008829       CO2        0.103179       H2O       0.097512       NO        0.005473       NO2       0.000036
     N2        0.733425       OH         0.000007       O2        0.051538

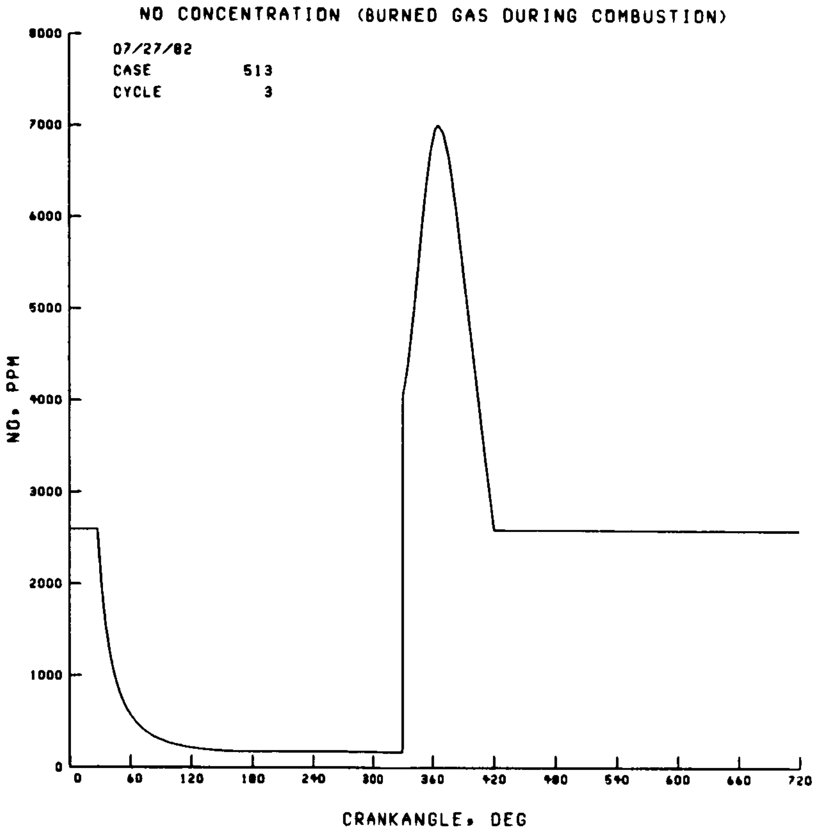
FRESH CHARGE MOLE FRACTIONS AT  244.07 K  AND  0.5264 ATM       MOLECULAR WEIGHT =  29.782
     C6H6      0.003375       C7H8       0.006040       C8H18     0.005385       AIR       0.985199

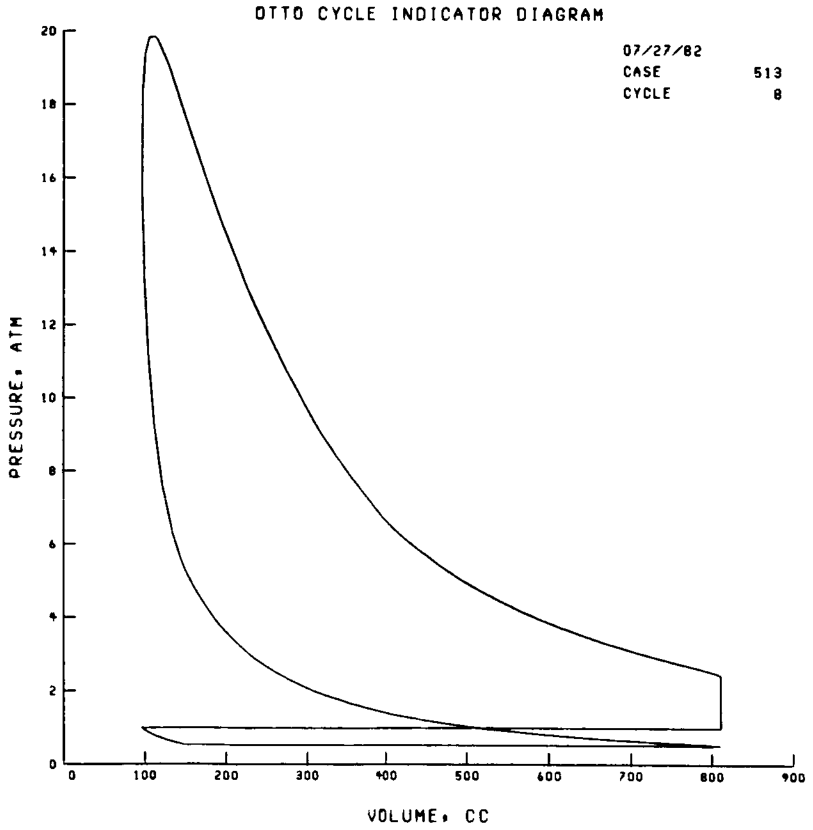
NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

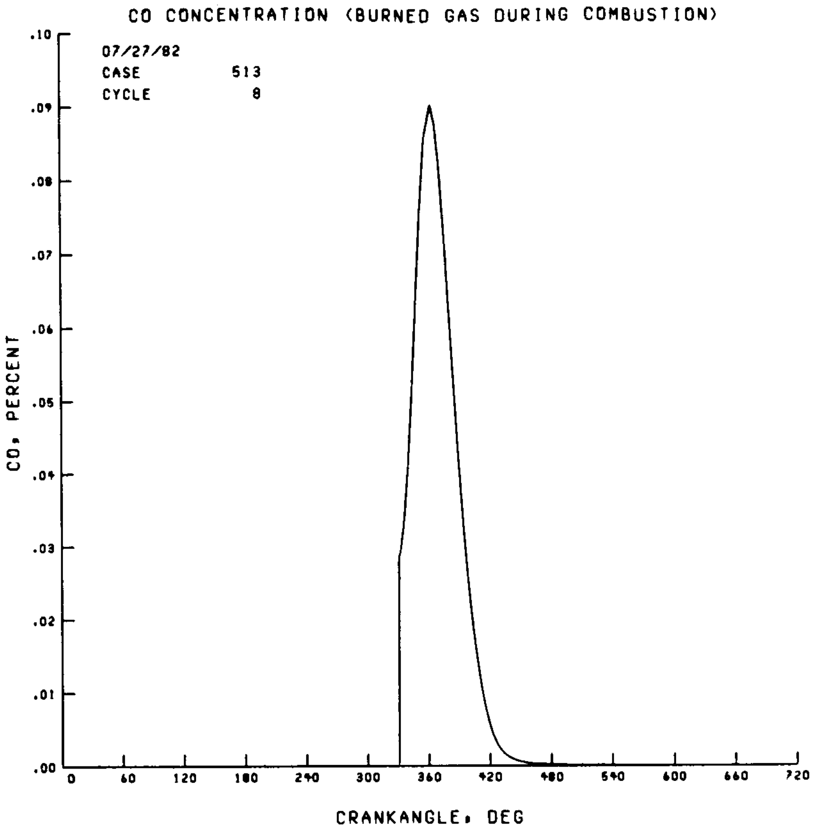
COMPUTER CYCLE TIME=   6.302 SEC
```

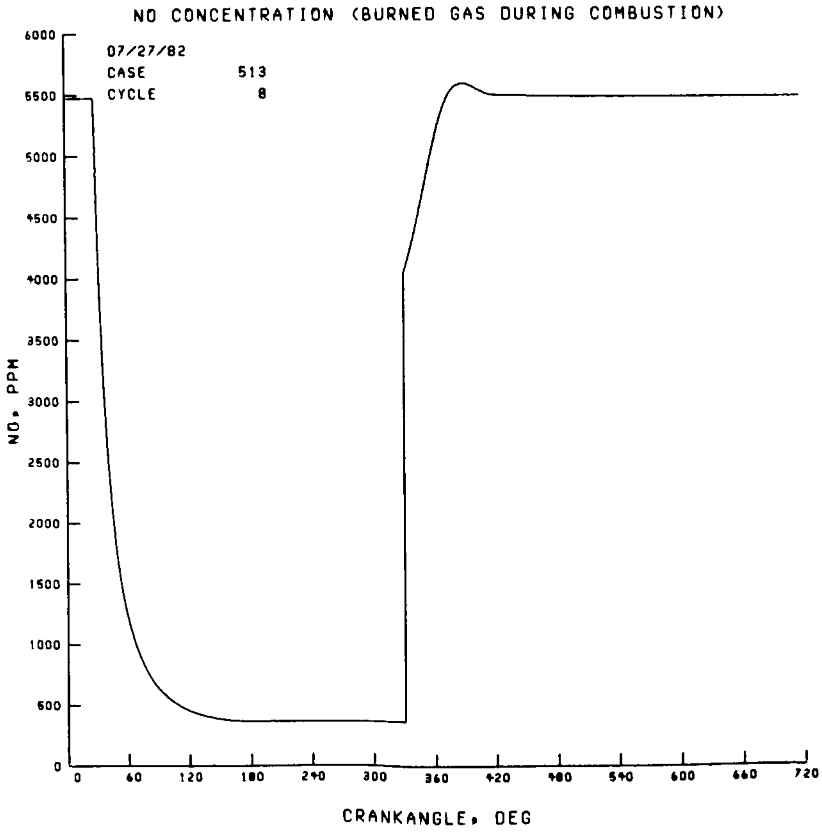

OTTO CYCLE INDICATOR DIAGRAM
07/27/82
CASE 513
CYCLE 3
PRESSURE, ATM
0
2
4
6
8
10
12
14
16
18
20
VOLUME, CC
0
100
200
300
400
500
600
700
800
900


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 513
CYCLE 3
CO, PERCENT
.00
.01
.02
.03
.04
.05
.06
.07
.08
.09
CRANKANGLE, DEG
0
60
120
180
240
300
360
420
480
540
600
660
720


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 513
CYCLE 3
NO, PPM
8000
7000
6000
5000
4000
3000
2000
1000
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


OTTO CYCLE INDICATOR DIAGRAM
07/27/82
CASE 513
CYCLE 8
PRESSURE, ATM
20
18
16
14
12
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
VOLUME, CC


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 513
CYCLE 8
CO, PERCENT
.10
.09
.08
.07
.06
.05
.04
.03
.02
.01
.00
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/27/82
CASE 513
CYCLE 8
NO, PPM
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

Appendix E

Example II (Case 1359)

Input, Case 1359

```
REAC
C 8.     H 18.                                .42              G298.15  F
C 7.     H 8.                                 .38              G298.15  F
C 6.     H 6.                                 .18              G298.15  F
C 8.     H 16.                                .02              G298.15  F

NAME
 &OTTINP FREQ=3500,BORE=10.922,STROKE=10.312,ROD=17.145,TW=360.,
 CA=129.03,CR=10.5,CSBURN=T,KASE=1359, PEXH=1.,PMFOLD=2.,
  HC3=0,HA=0,HB=0,HC2=0,
   &END
 &AFINP EQRAT=.9,SPARK=10.,EGR=.1,THBURN=30.,VARAF=F,IPRINT=6,
  IFLOW=5,NCYCLE=6&END
 &FLOWIN DIN=4.78155,DEX=3.65125,BETAIN=45,BETAEX=45,LIN=2.2,LINR=2.2,
  LEX=1.8,LEXR=1.8,AIN(1)=.95,AINR(1)=1.,AEXR(1)=.95,ALFAIN=0,ALFAEX=0,
  EIN(2)=-20,EINR(2)=-20,EEXR(2)=-15,EEX(2)=-15,EIN(3)=2,EINR(3)=2,
  EEXR(3)=2,EEX(3)=2,BIN(1)=.05,BINR(1)=.05,AEX(1)=1.,
  RIN=-1.2848969079444,-50.187346074604,1096.8283706756,-8957.6765334312,39006.948871083,
      -100238.56274839, 156517.07679742,-145707.72737296,74242.533537645,-15911.602212327,
  REX= -1.7570429627131, -29.707017135839, 740.07743781757, -5709.7197760822, 22840.404174765
  -53412.129620218, 75446.092321360, -63124.319964495, 28632.585430403, -5383.9560171224,
  IVOPEN=699,IVSHUT=265,EVOPEN=465,EVSHUT=45&END
```

Output, Case 1359

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                 CYCLE   5    LEVEL 1    CASE NO.     1359
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100      T(EGR) = 1112.0 K      SPARK ADVANCE =  10.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 2.00000 ATM      EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                    WT FRACTION   ENERGY   STATE    TEMP
           CHEMICAL FORMULA                                                       CAL/MOL           DEG K
FUEL     C  8.00000   H 18.00000                                      0.420000   -49910.473  G      298.15
FUEL     C  7.00000   H  8.00000                                      0.380000    11949.438  G      298.15
FUEL     C  6.00000   H  6.00000                                      0.180000    19818.801  G      298.15
FUEL     C  8.00000   H 16.00000                                      0.020000   -19814.664  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032            1.000000      -29.792  G      298.15

                  A/F= 15.7503   PERCENT FUEL=   5.9700   EQUIVALENCE RATIO= 0.9000   PHI=   0.8998
FUEL MASS FRACTION = 0.052653                 INDICATED MEAN EFFECTIVE PRESSURE (ATM) = 17.0038
AIR MASS FRACTION = 0.829307                  PUMP MEAN EFFECTIVE PRESSURE (ATM) =  1.0000
RESIDUAL MASS FRACTION = 0.020045             CHEMICAL ENERGY (JOULES/G) =2354.265
RECIRCULATED MASS FRACTION = 0.097995         MASS EFFICIENCY = 0.979955
MASS FRACTION EXHAUST RETAINED = 0.020033     VOLUME EFFICIENCY = 0.944477
NET WORK EFFICIENCY = 0.460386                FRACTIONAL MASS CHANGE 6 - 7 =-0.789651

THERMODYNAMIC PROPERTIES

STATION                        2         3         4         5         6         7
CRANKANGLE        0.0000    0.0000    180.00    350.00    350.00    540.00    540.00    0.0000
P, ATM            2.0000    2.0000    2.0000    38.734    118.27    7.3110    1.0000    1.0000
T, DEG K           463.4     759.4     482.0     972.3    2854.3    1711.0    1112.6     298.1
RHO, G/CC       1.5847-3 9.5739-4 1.5228-3 1.4620-2 1.4620-2 1.5228-3 3.2033-4 1.2886-3
H, CAL/G         -24.660   -124.44   -30.634    107.16    238.92   -190.83   -379.27   -639.72
U, CAL/G         -55.224   -175.03   -62.439    43.001    43.001   -307.09   -454.87   -658.51
S, CAL/(G)(K)     1.6610    1.8418    1.6752    1.6752    2.0028    2.0028    2.0028    1.5588
CP, CAL/(G)(K)    0.2584    0.2831    0.2600    0.2999    0.5076    0.3271    0.3025    0.9115
GAMMA (S)         1.3427    1.3077    1.3401    1.2822    1.1878    1.2627    1.2897    1.1604
M, MOL WT         30.131    29.828    30.112    30.112    28.951    29.245    29.245    31.526

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR               0.00092  0.00364  0.00108  0.00108  0.00880  0.00889  0.00889  0.00889
CO               0.00000  0.00001  0.00000  0.00000  0.01397  0.00003  0.00003  0.00000
CO2              0.01325  0.05265  0.01563  0.01563  0.11342  0.12866  0.12866  0.12869
H                0.00000  0.00000  0.00000  0.00000  0.00037  0.00000  0.00000  0.00000
HO2              0.00000  0.00000  0.00000  0.00000  0.00003  0.00000  0.00000  0.00000
H2               0.00000  0.00000  0.00000  0.00000  0.00168  0.00001  0.00001  0.00000
H2O(L)           0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.07232
H2O              0.01041  0.04136  0.01228  0.01228  0.09508  0.10106  0.10106  0.02882
NO               0.00126  0.00501  0.00149  0.00149  0.01211  0.01223  0.01223  0.00000
NO2              0.00000  0.00000  0.00000  0.00000  0.00002  0.00000  0.00000  0.00000
N2               0.07575  0.30092  0.08936  0.08936  0.72781  0.73520  0.73520  0.74135
O                0.00000  0.00000  0.00000  0.00000  0.00086  0.00000  0.00000  0.00000
OH               0.00001  0.00005  0.00002  0.00002  0.00632  0.00012  0.00012  0.00000
O2               0.00143  0.00566  0.00168  0.00168  0.01954  0.01379  0.01379  0.01992
C6H6             0.00373  0.00246  0.00365  0.00365  0.00000  0.00000  0.00000  0.00000
C7H8             0.00668  0.00440  0.00654  0.00654  0.00000  0.00000  0.00000  0.00000
C8H16            0.00029  0.00019  0.00028  0.00028  0.00000  0.00000  0.00000  0.00000
C8H18            0.00595  0.00392  0.00583  0.00583  0.00000  0.00000  0.00000  0.00000
```

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   4    LEVEL 2    CASE NO.     1359
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.100     T(EGR) =  965.8 K     SPARK ADVANCE =  10.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 2.00000 ATM     EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN =   0.00 DEG     IVSHUT = 180.00 DEG                         EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 29.8 DEG    COSINE  COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.500000  -0.500000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  8.00000   H 18.00000                                                0.420000   -49910.473   G    298.15
FUEL    C  7.00000   H  8.00000                                                0.380000    11949.438   G    298.15
FUEL    C  6.00000   H  6.00000                                                0.180000    19818.801   G    298.15
FUEL    C  8.00000   H 16.00000                                                0.020000   -19814.664   G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792   G    298.15

                  A/F= 15.7503   PERCENT FUEL=   5.9700   EQUIVALENCE RATIO= 0.9000    PHI=   0.8998

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL       1.72282                      CHARGE      49.0332                        EXHAUST     49.0329
     FUEL        0.09033                      FUEL          2.6346                       CO          0.00008
     AIR         1.42270                      AIR         41.4953                        NOX         0.45810

   ENERGY PER CYCLE (JOULES)             AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK        1698.844           INDICATED POWER         49.550                NET WORK      0.444992
 INDICATED PUMP WORK     97.891           INDICATED PUMP POWER     2.855                HEAT LOSS     0.114674
 HEAT LOSS              463.015           HEAT LOSS RATE          13.505                EXHAUST       0.378515
 CHEM. ENERGY          4037.678           EXHAUST POWER           44.576
                                                    MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)           17.3540
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                  1.0000
                               MEAN TORQUE (NEWTON-METERS)                      142.9796

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  965.61 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  29.246
     AR        0.008891      CO2      0.128694      H2O      0.101127      NO       0.009104      N2       0.736795
     OH        0.000024      O2       0.015360

FRESH CHARGE MOLE FRACTIONS AT  443.64 K  AND  2.0000 ATM      MOLECULAR WEIGHT =  30.131
     AR        0.000916      CO2      0.013259      H2O      0.010419      NO       0.000938      N2       0.075908
     O2        0.001582      C6H6     0.003731      C7H8     0.006677      C8H16    0.000289      C8H18    0.005952
     AIR       0.880326

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   2.207 SEC
```

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE   6    LEVEL 4    CASE NO.     1359
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100      T(EGR) =  966.4 K      SPARK ADVANCE =  10.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 2.00000 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                  EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME     FINITE BURNING INTERVAL = 29.8 DEG    COSINE  COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.500000  -0.500000

                                                                                  WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                       CAL/MOL           DEG K
FUEL     C  8.00000   H 18.00000                                                     0.420000   -49910.473  G     298.15
FUEL     C  7.00000   H  8.00000                                                     0.380000    11949.438  G     298.15
FUEL     C  6.00000   H  6.00000                                                     0.180000    19818.801  G     298.15
FUEL     C  8.00000   H 16.00000                                                     0.020000   -19814.664  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                           1.000000      -29.792  G     298.15

                     A/F= 15.7503   PERCENT FUEL=   5.9700   EQUIVALENCE RATIO= 0.9000   PHI=   0.8998

                                            PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                         MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         1.55318                           CHARGE        43.2434                        EXHAUST        44.7788
     FUEL          0.07951                           FUEL           2.3235                        CO              0.00009
     AIR           1.25224                           AIR           36.5956                        NOX             0.39406
                                                     NET           43.2316                        NET            44.7782

   ENERGY PER CYCLE (JOULES)                    AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK         1490.519              INDICATED POWER          43.473                NET WORK       0.390356
 INDICATED PUMP WORK    -101.246              INDICATED PUMP POWER     -2.953                HEAT LOSS      0.132943
 HEAT LOSS               473.144              HEAT LOSS RATE           13.800                EXHAUST        0.385880
 CHEM. ENERGY           3558.992              EXHAUST POWER            40.056

                                                         MISCELLANEOUS

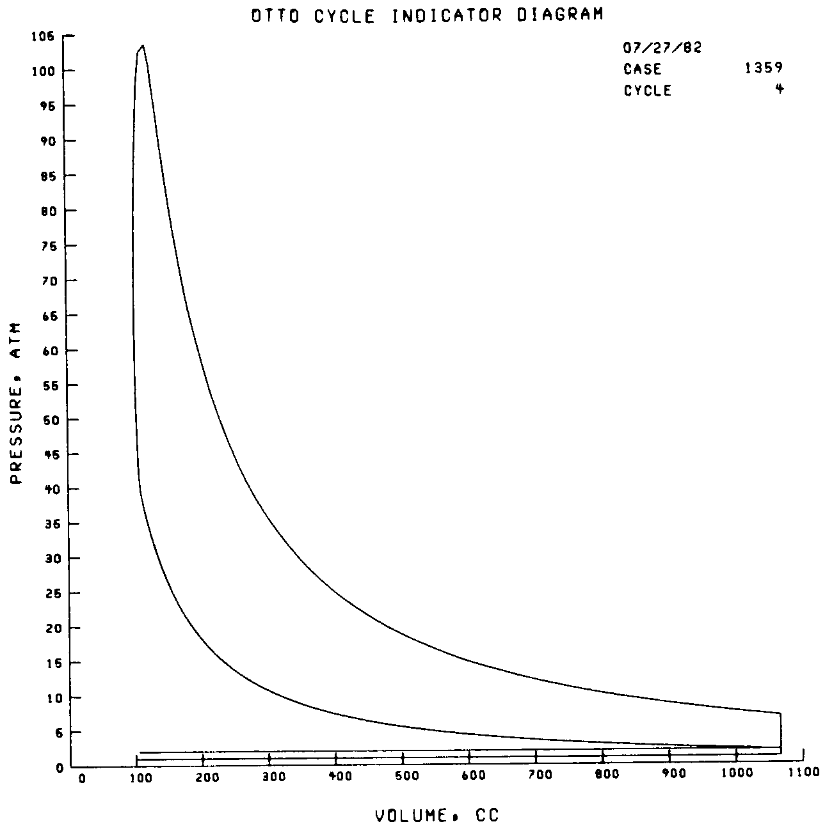
                                  INDICATED MEAN EFFECTIVE PRESSURE (ATM)              15.2260
                                  PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -1.0342
                                  MEAN TORQUE (NEWTON-METERS)                          110.5548

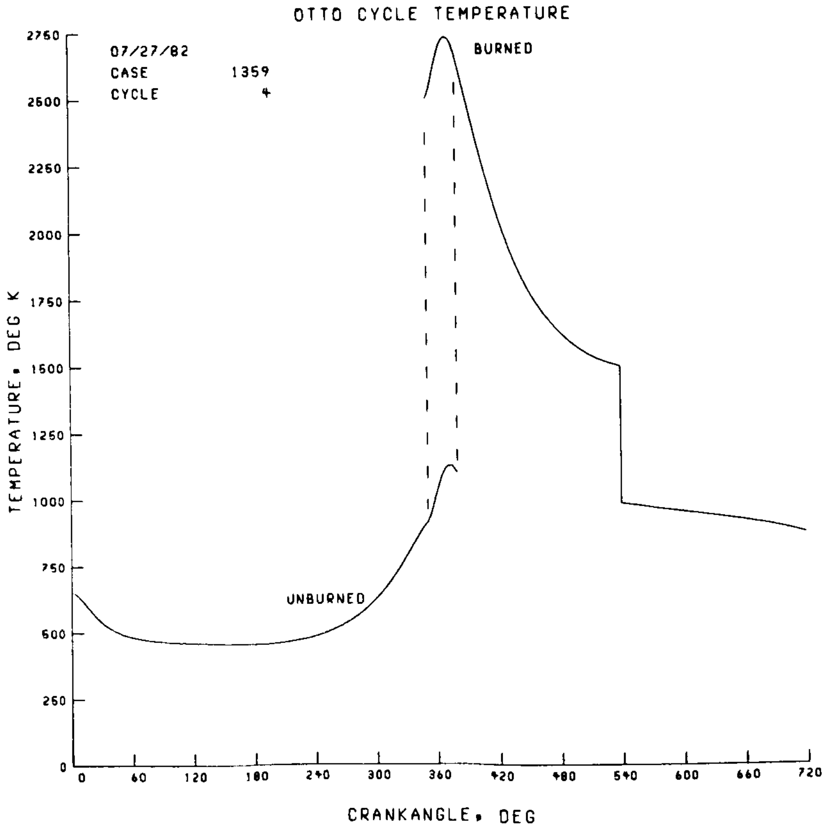
COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  966.38 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  29.246
     AR        0.008887       CO2        0.128633       H2O       0.101086       NO        0.008518       NO2        0.000038
     N2        0.736712       OH         0.000010       O2        0.015610       AIR       0.000492

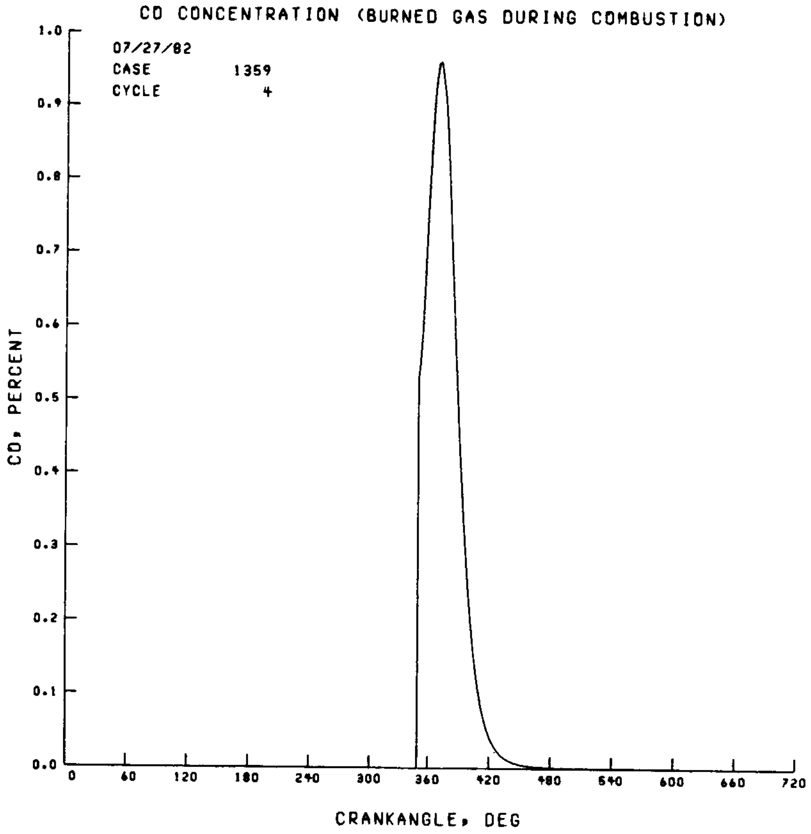
FRESH CHARGE MOLE FRACTIONS AT  443.72 K  AND  2.0000 ATM      MOLECULAR WEIGHT =  30.131
     AR        0.000916       CO2        0.013252       H2O       0.010414       NO        0.000878       N2         0.075899
     O2        0.001608       C6H6       0.003731       C7H8      0.006677       C8H16     0.000289       C8H18      0.005953
     AIR       0.880378

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

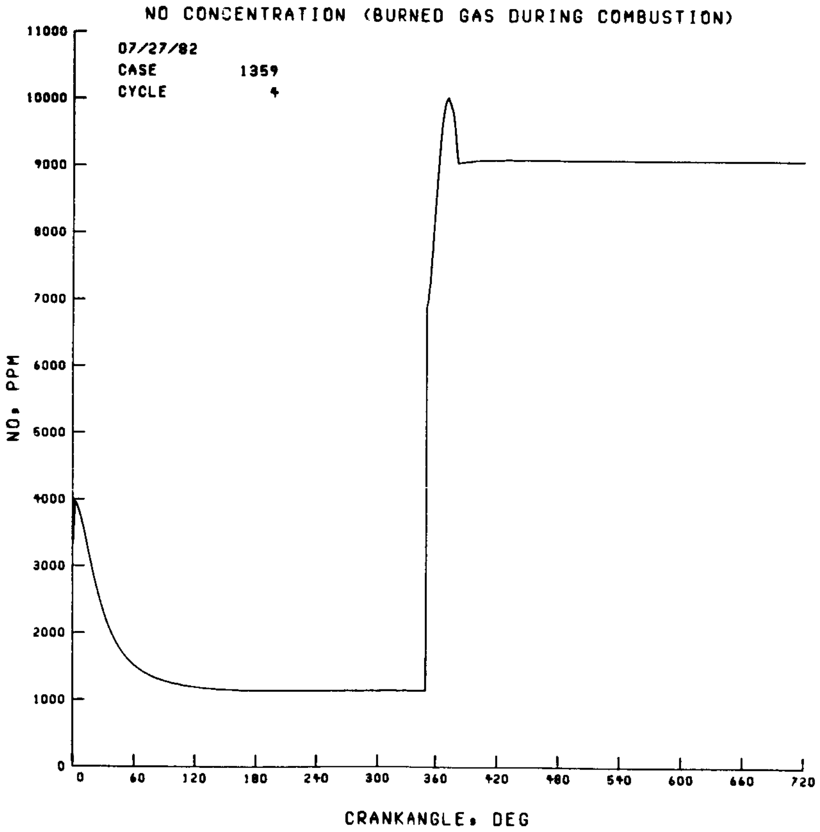
COMPUTER CYCLE TIME=  11.554 SEC
```


OTTO CYCLE INDICATOR DIAGRAM
07/27/82
CASE 1359
CYCLE 4
PRESSURE, ATM
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
VOLUME, CC
0
100
200
300
400
500
600
700
800
900
1000
1100

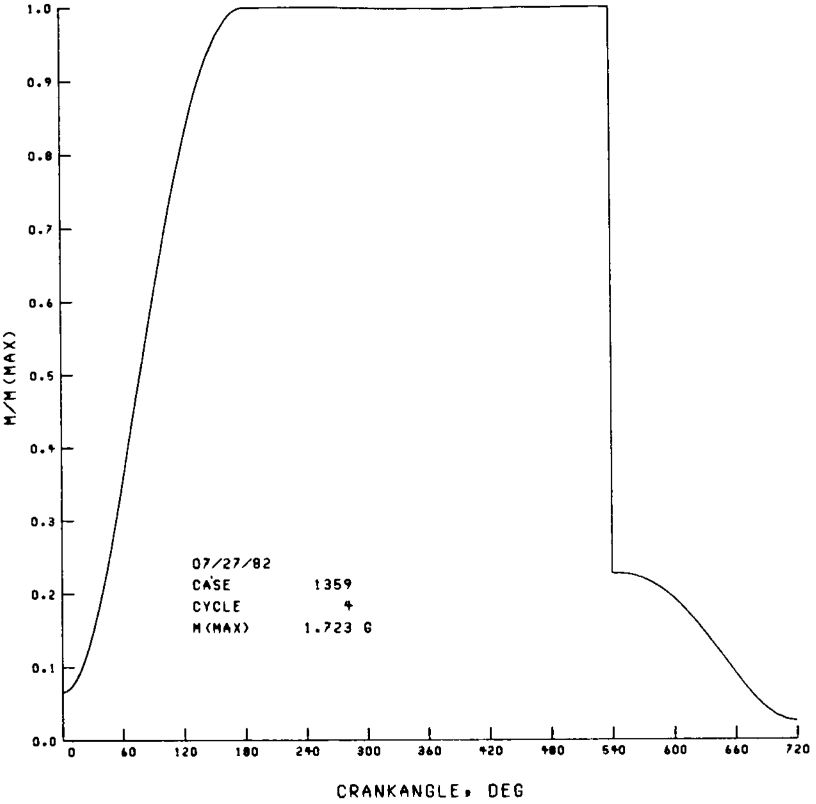

OTTO CYCLE TEMPERATURE
07/27/82
CASE 1359
CYCLE 4
BURNED
UNBURNED
TEMPERATURE, DEG K
0
250
500
750
1000
1250
1500
1750
2000
2250
2500
2750
CRANKANGLE, DEG
0
60
120
180
240
300
360
420
480
540
600
660
720


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)

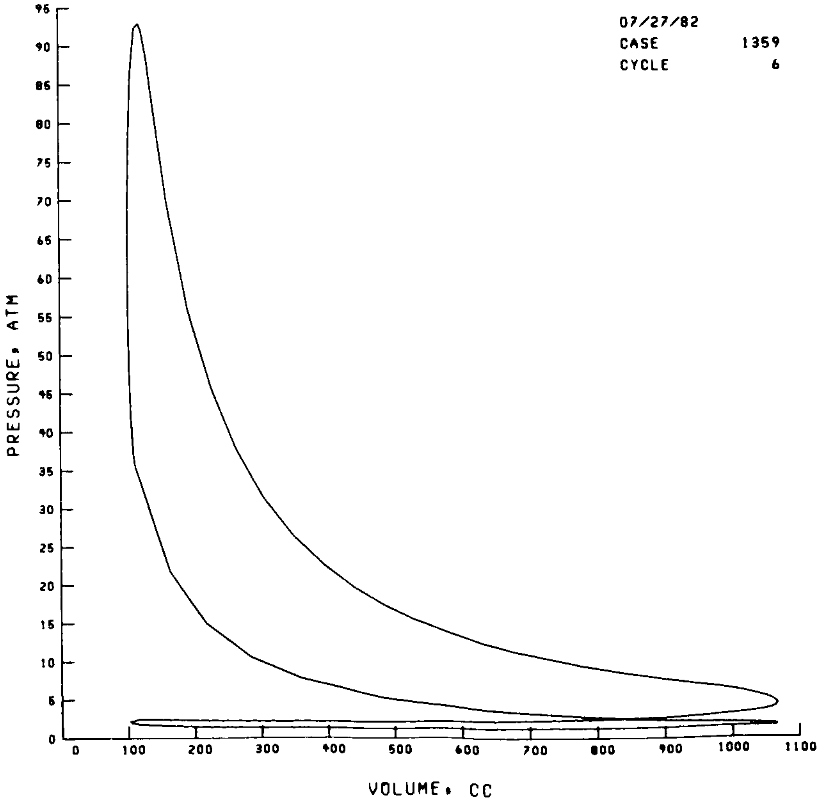
07/27/82
CASE 1359
CYCLE 4


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)

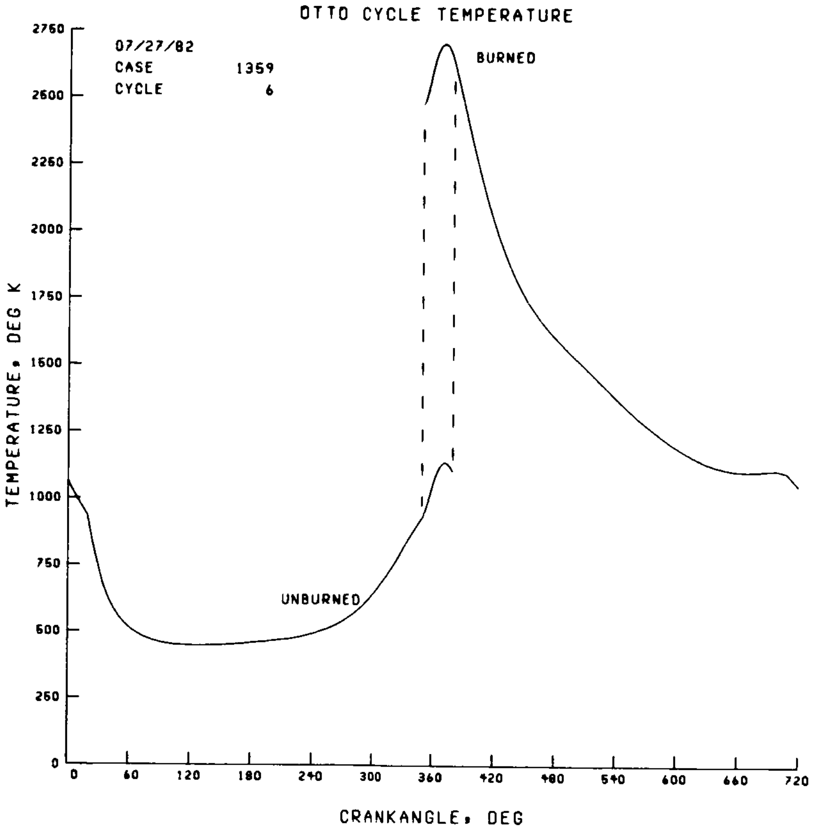
07/27/82
CASE 1359
CYCLE 4



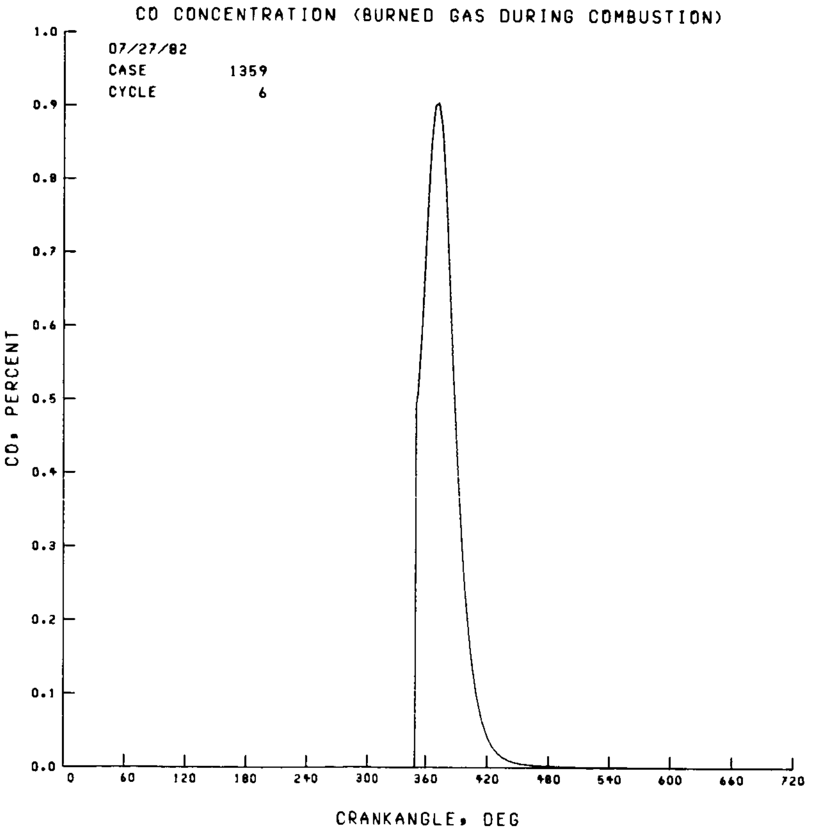
OTTO CYCLE MASS



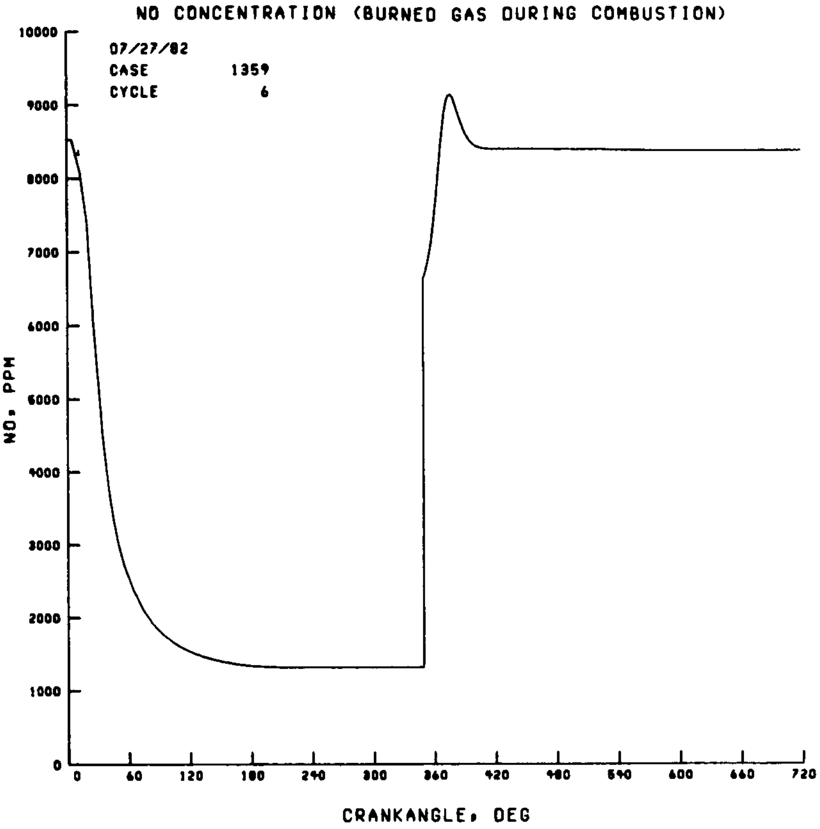
OTTO CYCLE INDICATOR DIAGRAM



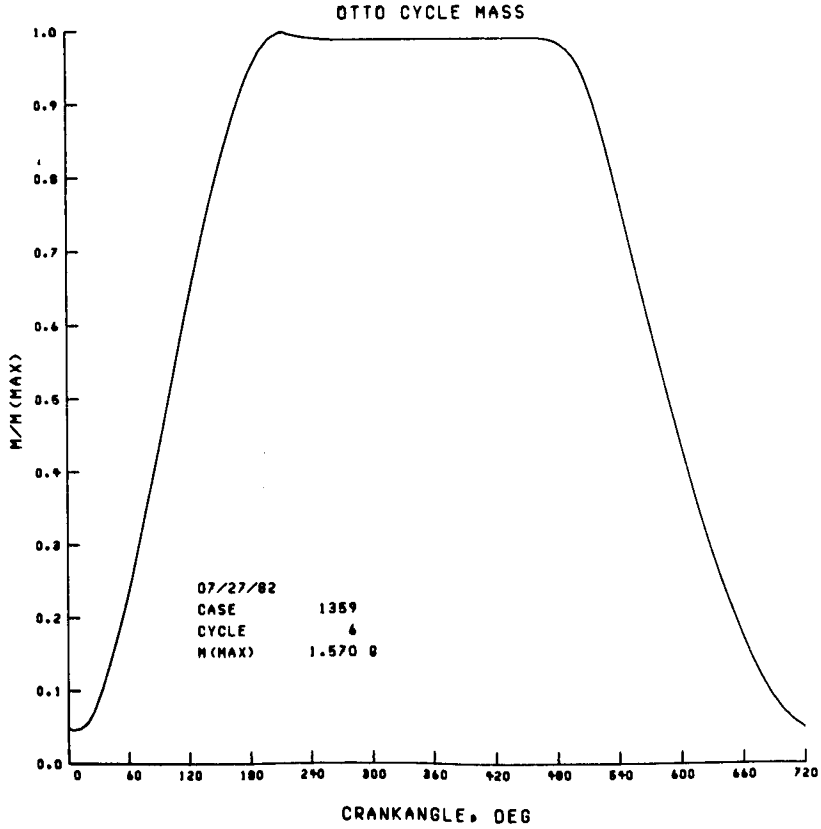
OTTO CYCLE TEMPERATURE



CO CONCENTRATION (BURNED GAS DURING COMBUSTION)


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)

07/27/82
CASE 1359
CYCLE 6


OTTO CYCLE MASS

07/27/82
CASE 1359
CYCLE 6
M(MAX) 1.570 G

Output, Case 13591

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   6    LEVEL 4    CASE NO.    13591
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100     T(EGR) =  675.0 K     SPARK ADVANCE =  10.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 2.00000 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                               EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS    C1 =      0.000000    C2 = 0.387200E 00    C3 =      0.000000     A =  0.4000     B =  0.8000

EQUILIBRIUM FLAME     FINITE BURNING INTERVAL = 29.8 DEG    COSINE   COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.500000  -0.500000

                                                                                  WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                        CAL/MOL           DEG K
FUEL     C  8.00000   H 18.00000                                                    0.420000    -49910.473  G     298.15
FUEL     C  7.00000   H  8.00000                                                    0.380000     11949.438  G     298.15
FUEL     C  6.00000   H  6.00000                                                    0.180000     19818.801  G     298.15
FUEL     C  8.00000   H 16.00000                                                    0.020000    -19814.664  G     298.15
AIR      N  1.56168   O  0.41959    AR 0.00936    C  0.00032                        1.000000       -29.792  G     298.15

                          A/F= 15.7503    PERCENT FUEL=    5.9700   EQUIVALENCE RATIO= 0.9000    PHI=    0.8998

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                         MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          1.81510                            CHARGE        50.4332                        EXHAUST       50.7798
     FUEL           0.09272                            FUEL           2.7098                        CO            0.00003
     AIR            1.46035                            AIR           42.6801                        NOX           0.30952
                                                       NET           50.4162                        NET           50.7790

   ENERGY PER CYCLE (JOULES)                    AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK         1282.396               INDICATED POWER          37.403                  NET WORK      0.302981
 INDICATED PUMP WORK     -25.875               INDICATED PUMP POWER     -0.755                  HEAT LOSS     0.429799
 HEAT LOSS              1782.459               HEAT LOSS RATE           51.988                  EXHAUST       0.226245
 CHEM. ENERGY           4147.188               EXHAUST POWER            27.366

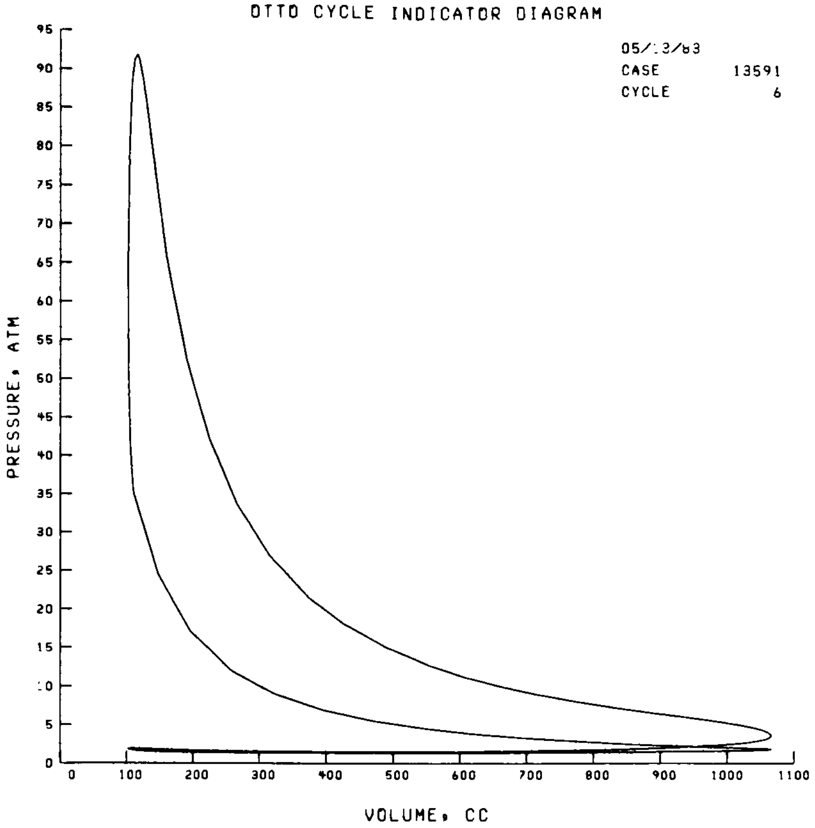
                                                              MISCELLANEOUS

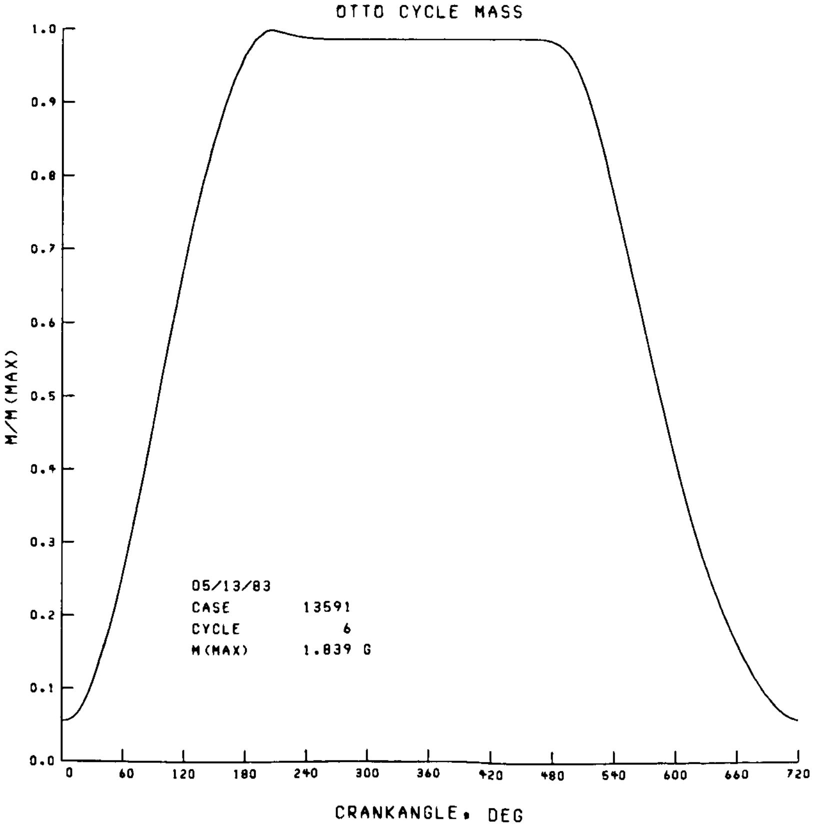
                                       INDICATED MEAN EFFECTIVE PRESSURE (ATM)                 13.0999
                                       PUMP MEAN EFFECTIVE PRESSURE (ATM)                      -0.2643
                                       MEAN TORQUE (NEWTON-METERS)                             99.9906

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  674.98 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  29.247
     AR        0.008881      CO2       0.128579      H2O       0.101028      NO        0.005870      NO2       0.000046
     N2        0.737498      O2        0.016897      C6H6      0.000005      C7H8      0.000010      C8H18     0.000009
     AIR       0.001176

FRESH CHARGE MOLE FRACTIONS AT  405.43 K  AND  2.0000 ATM      MOLECULAR WEIGHT =  30.131
     AR        0.000915      CO2       0.013246      H2O       0.010408      NO        0.000605      N2        0.075978
     O2        0.001741      C6H6      0.003731      C7H8      0.006678      C8H16     0.000289      C8H18     0.005953
     AIR       0.880450

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.
```


OTTO CYCLE INDICATOR DIAGRAM
05/13/83
CASE 13591
CYCLE 6
PRESSURE, ATM
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
VOLUME, CC
0
100
200
300
400
500
600
700
800
900
1000
1100


OTTO CYCLE MASS
M/M(MAX)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
05/13/83
CASE 13591
CYCLE 6
M(MAX) 1.839 G
CRANKANGLE, DEG
0
60
120
180
240
300
360
420
480
540
600
660
720

Appendix F

Example III (Case 99)

Input, Case 99

```
REAC
C 3.     H 8.                                  1.              G298.15  F

NAME
 &OTTINP FREQ=3500,BORE=10.922,STROKE=10.312,ROD=17.145,CA=129.03,
 TW=360.,CR=10.5,KASE=99,
 PEXH=1.,PMFOLD=.4276,
 HC3=0.,HA=.4,HB=.8,HC2=.3872,
   SP=T,RHUMID=75.,TAIR=298.15&END
 &AFINP DEBUG=T,EQRAT=1.,THBURN=0.,
 KINET=3,NCYCLE=8,IFLOW=5,VARAF=F&END
 &FLOWIN DIN=4.78155,DEX=3.65125,BETAIN=45,BETAEX=45,LIN=2.2,LINR=2.2,
  LEX=1.8,LEXR=1.8,AIN(1)=.95,AINR(1)=1.,AEXR(1)=.95,
  EIN(2)=-20,EINR(2)=-20,EEXR(2)=-15,EEX(2)=-15,EIN(3)=2,EINR(3)=2,
  EEXR(3)=2,EEX(3)=2,BIN(1)=.05,BINR(1)=.05,AEX(1)=1.,
  RIN=.11655397536916,-1.2305226637252,53.276925905521,-329.46664003586,967.59957726191,
  -1606.5917666613,1531.2782499752,-777.72614964883,162.74377189163,
  REX=.015239819814648,1.2692256549564,24.316014460188,-83.715719936202,
  -146.81709604486,1257.7189438064,-2839.5867388125,3151.0342473402,
  -1758.248769365,394.01465307699,POLY=T
  IVOPEN=699,IVSHUT=265,EVOPEN=465,EVSHUT=45&END
```

Output, Case 99

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                  CYCLE  11    LEVEL 1    CASE NO.        99
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.000      T(EGR) =  298.1 K      SPARK ADVANCE =    0.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                        WT FRACTION   ENERGY    STATE    TEMP
          CHEMICAL FORMULA                                                            CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                          1.000000    -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032               *1.000000     -1386.340  G     298.15
                   * AIR INCLUDES   0.02348 MOLE FRACTION WATER         RELATIVE HUMIDITY= 0.7500

                  A/F= 15.9132   PERCENT FUEL=   5.9125   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000
FUEL MASS FRACTION = 0.048666                            INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  0.0000
AIR MASS FRACTION = 0.774425                             PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.5527
RESIDUAL MASS FRACTION = 0.176910                        CHEMICAL ENERGY (JOULES/G) =2967.627
RECIRCULATED MASS FRACTION = 0.000000                    MASS EFFICIENCY = 0.823090
MASS FRACTION EXHAUST RETAINED = 0.176914                VOLUME EFFICIENCY = 0.823087
NET WORK EFFICIENCY =-0.026474                           FRACTIONAL MASS CHANGE 6 - 7 = 0.857599

THERMODYNAMIC PROPERTIES

STATION                           2          3          4          5          6          7
CRANKANGLE           0.0000    30.787     180.00     360.00     360.00     540.00     540.00     0.0000
P, ATM               0.4276    0.4276     0.4276     10.343     10.343     0.4276     1.0000     1.0000
T, DEG K              236.8     236.8      236.8      545.6      545.6      236.8      298.1      298.1
RHO, G/CC          6.4497-4  6.4496-4   6.4497-4   6.7722-3   6.7722-3   6.4497-4   1.1981-3   1.3505-3
H, CAL/G            -94.061   -93.976    -94.046    -13.561    -13.561    -94.046    -78.670    -787.98
U, CAL/G            -110.12   -110.03    -110.10    -50.549    -50.549    -110.10    -98.883    -805.91
S, CAL/(G)(K)        1.6165    1.6165     1.6165     1.6165     1.6165     1.6165     1.6165     1.5251
CP, CAL/(G)(K)       0.2482    0.2482     0.2482     0.2752     0.2752     0.2482     0.2524     0.9203
GAMMA (S)            1.3757    1.3758     1.3758     1.3268     1.3268     1.3758     1.3673     1.1480
M, MOL WT            29.313    29.311     29.312     29.312     29.312     29.312     29.312     33.041

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR                  0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.00845
CO2                 0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.11368
H2O(L)              0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.14638
H2O                 0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.02652
N2                  0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.70486
O2                  0.00000   0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.00010
C3H8                0.03930   0.03919    0.03928    0.03928    0.03928    0.03928    0.03924    0.00000
AIR                 0.96070   0.96081    0.96072    0.96072    0.96072    0.96072    0.96076    0.00000


TOTAL COMPUTER TIME=   1.149 SEC        DELTA TIME =  0.074 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE    4    LEVEL 2    CASE NO.       99
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.000     T(EGR) =  298.1 K      SPARK ADVANCE =    0.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =   966.13 CC

IVOPEN =  31.45 DEG     IVSHUT = 180.00 DEG                         EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

         NO FLAME    FINITE BURNING INTERVAL =  0.0 DEG    LINEAR  COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000

                                                                             WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                  CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                 1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      *1.000000    -1386.340  G    298.15
                 * AIR INCLUDES   0.02348 MOLE FRACTION WATER               RELATIVE HUMIDITY= 0.7500

                  A/F= 15.9132   PERCENT FUEL=   5.9125   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.63050                       CHARGE      15.2254                       EXHAUST      30.8093
     FUEL          0.03086                       FUEL         0.9002                       CO           0.00000
     AIR           0.49115                       AIR         14.3252                       NOX          0.00000

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK          -11.842       INDICATED POWER          -0.345               NET WORK      -0.035193
 INDICATED PUMP WORK     -54.036       INDICATED PUMP POWER     -1.576               HEAT LOSS     -0.003682
 HEAT LOSS                -6.892       HEAT LOSS RATE           -0.201               EXHAUST        1.693001
 CHEM. ENERGY           1871.925       EXHAUST POWER            92.434
                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              -0.1210
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -0.5520
                              MEAN TORQUE (NEWTON-METERS)                          -5.2424

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  336.10 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  29.313
     C3H8      0.039297      AIR        0.960702

FRESH CHARGE MOLE FRACTIONS AT  236.83 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.313
     C3H8      0.039303      AIR        0.960696

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   1.145 SEC
```

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                  CYCLE   8    LEVEL 4    CASE NO.       99
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =   0.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                       EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

         NO FLAME    FINITE BURNING INTERVAL =  0.0 DEG    LINEAR  COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000

                                                                         WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                               CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                            1.000000    -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                 *1.000000     -1386.340  G     298.15
                    * AIR INCLUDES   0.02348 MOLE FRACTION WATER         RELATIVE HUMIDITY= 0.7500

                  A/F= 15.9132   PERCENT FUEL=   5.9125   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)      MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.56826                       CHARGE        8.2279                  EXHAUST      18.5673
     FUEL         0.03360                       FUEL          0.4865                  CO            0.00000
     AIR          0.53466                       AIR           7.7414                  NOX           0.00000
                                                NET           8.2308                  NET           8.2614

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)             CYCLE EFFICIENCIES

 INDICATED WORK          -10.672         INDICATED POWER          -0.311            NET WORK      -0.073750
 INDICATED PUMP WORK    -113.758         INDICATED PUMP POWER     -3.318            HEAT LOSS      0.002430
 HEAT LOSS                 4.100         HEAT LOSS RATE            0.120            EXHAUST        1.137793
 CHEM. ENERGY           1687.191         EXHAUST POWER            55.990

                                                   MISCELLANEOUS

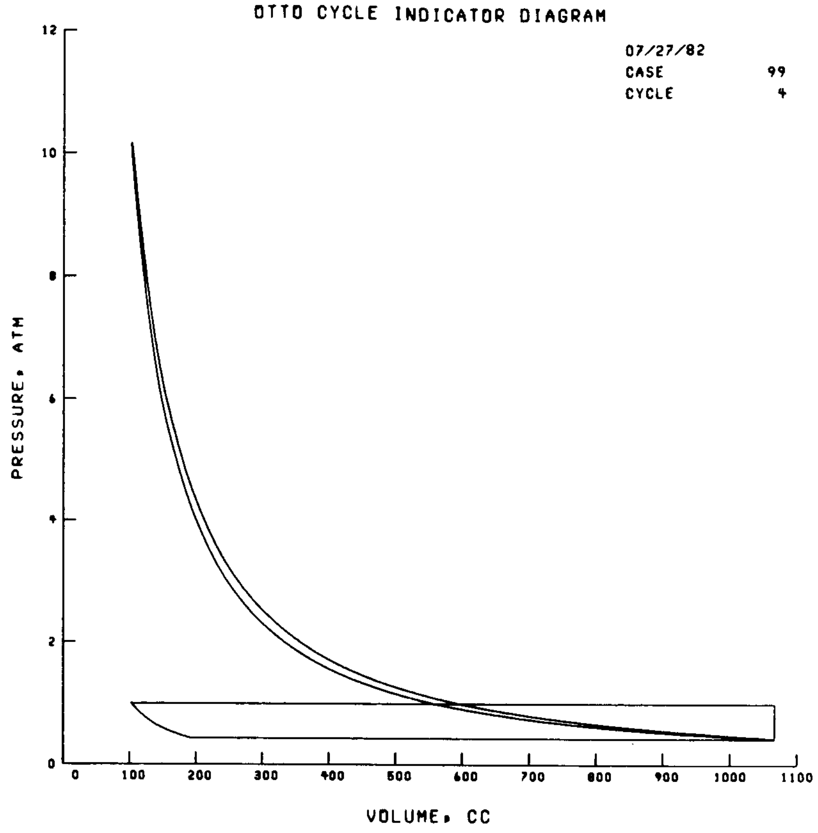
                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)               -0.1090
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -1.1621
                              MEAN TORQUE (NEWTON-METERS)                           -9.9018

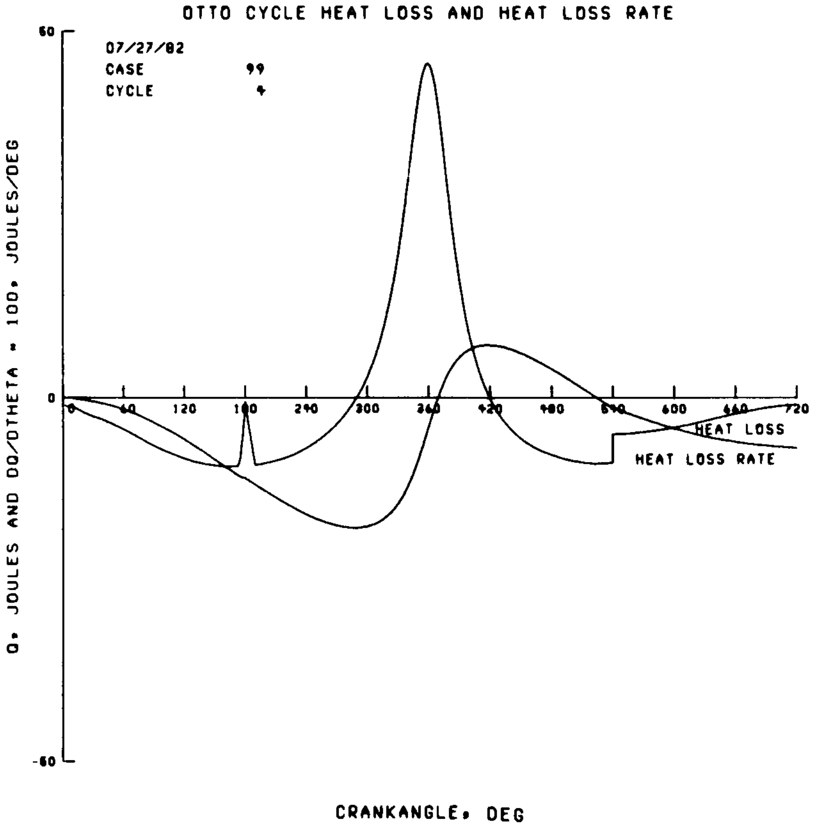
COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  341.91 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  29.313
     C3H8      0.039302       AIR        0.960698

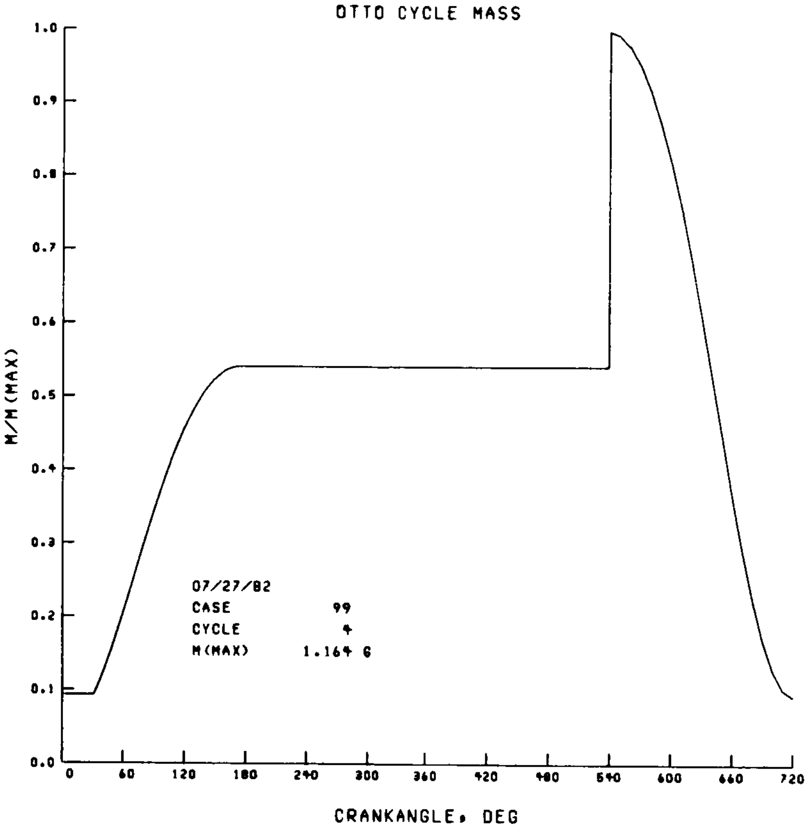
FRESH CHARGE MOLE FRACTIONS AT  236.83 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.313
     C3H8      0.039303       AIR        0.960696

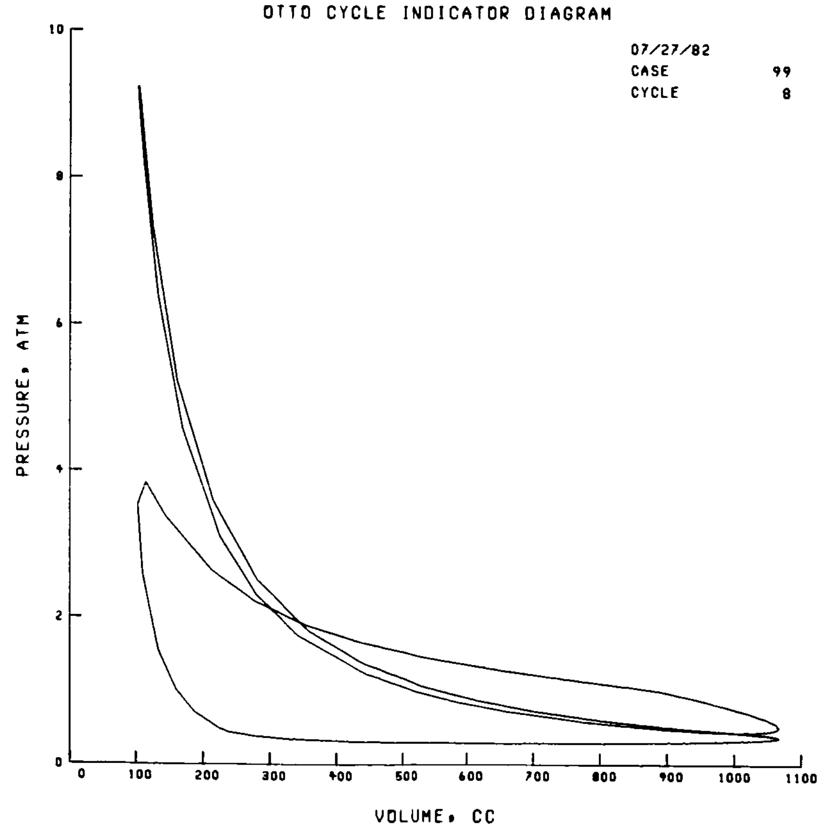
NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

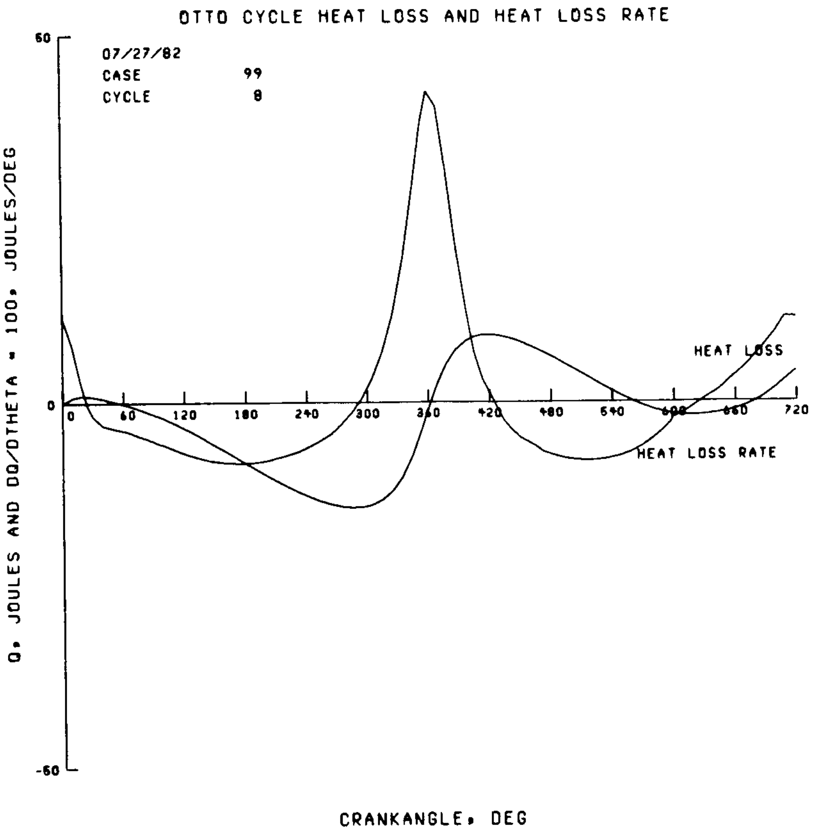
COMPUTER CYCLE TIME=  14.918 SEC
```

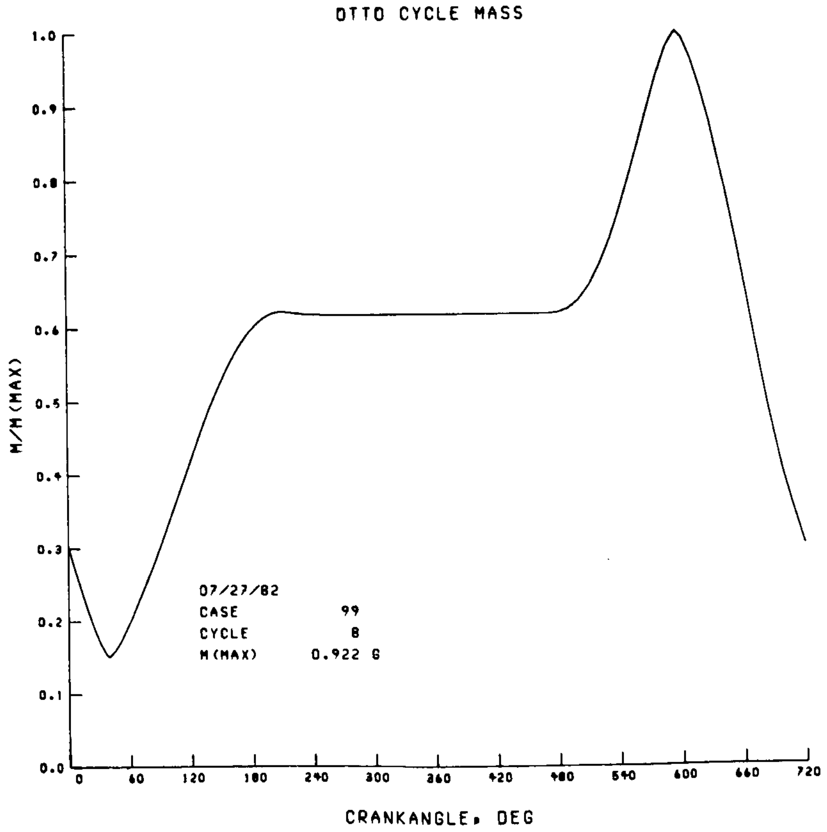

OTTO CYCLE INDICATOR DIAGRAM


OTTO CYCLE HEAT LOSS AND HEAT LOSS RATE


OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
07/27/82
CASE 99
CYCLE 4
M(MAX) 1.164 G
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


OTTO CYCLE INDICATOR DIAGRAM
07/27/82
CASE 99
CYCLE 8
PRESSURE, ATM
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
1000
1100
VOLUME, CC


OTTO CYCLE HEAT LOSS AND HEAT LOSS RATE
07/27/82
CASE 99
CYCLE 8
Q, JOULES AND DQ/DTHETA * 100, JOULES/DEG
60
0
-60
0
60
120
180
240
300
360
420
480
540
600
660
720
HEAT LOSS
HEAT LOSS RATE
CRANKANGLE, DEG


OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
07/27/82
CASE 99
CYCLE 8
M(MAX) 0.922 G
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

Appendix G

Example IV (Case 111)

Input, Case 111

```
REAC
C 3.     H 8.                                1.             G298.15  F

NAME
 &OTTINP FREQ=3500,BORE=10.922,STROKE=10.312,ROD=17.145,CA=129.03,
 TW=360.,CR=10.5,BETA=3.2,KASE=111,
 PEXH=1.,PMFOLD=.4276,
 HC3=0.,HA=.4,HB=.8,HC2=.3872,
   SP=T,RHUMID=75.,TAIR=298.15&END
 &AFINP DEBUG=T,EQRAT=1.25,SPARK=20.,EGR=.1,THBURN=110.,
 NCYCLE=15,TAU=8.93E-05,IFLOW=3,VARAF=F,KFLAME=3&END
 &FLOWIN DIN=4.78155,DEX=3.65125,BETAIN=45,BETAEX=45,LIN=2.2,LINR=2.2,
  LEX=1.8,LEXR=1.8,AIN(1)=.95,AINR(1)=1.,AEXR(1)=.95,
  EIN(2)=-20,EINR(2)=-20,EEXR(2)=-15,EEX(2)=-15,EIN(3)=2,EINR(3)=2,
  EEXR(3)=2,EEX(3)=2,BIN(1)=.05,BINR(1)=.05,AEX(1)=1.,
  RIN=.11655397536916,-1.2305226637252,53.276925905521,-329.46664003586,967.59957726191,
  -1606.5917666613,1531.2782499752,-777.72614964883,162.74377189163,
  REX=.015239819814648,1.2692256549564,24.316014460188,-83.715719936202,
  -146.81709604486,1257.7189438064,-2839.5867388125,3151.0342473402,
  -1758.248769365,394.01465307699,POLY=T,
  IVOPEN=699,IVSHUT=265,EVOPEN=465,EVSHUT=45&END
```

Output, Case 111

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE   6    LEVEL 1    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100      T(EGR) = 1348.1 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM       EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                             WT FRACTION   ENERGY   STATE    TEMP
          CHEMICAL FORMULA                                                                CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                               1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                    *1.000000    -1386.340  G     298.15
                  * AIR INCLUDES   0.02348 MOLE FRACTION WATER               RELATIVE HUMIDITY= 0.7500

                  A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647
FUEL MASS FRACTION = 0.062311                        INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  4.0260
AIR MASS FRACTION = 0.784012                         PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.5512
RESIDUAL MASS FRACTION = 0.059641                    CHEMICAL ENERGY (JOULES/G) =2631.753
RECIRCULATED MASS FRACTION = 0.094036                MASS EFFICIENCY = 0.940359
MASS FRACTION EXHAUST RETAINED = 0.059645            VOLUME EFFICIENCY = 0.815920
NET WORK EFFICIENCY = 0.313333                       FRACTIONAL MASS CHANGE 6 - 7 =-0.373728

THERMODYNAMIC PROPERTIES

STATION                          2        3        4        5        6        7
CRANKANGLE          0.0000   32.169   180.00   340.00   340.00   540.00   540.00   0.0000
P, ATM              0.4276   0.4276   0.4276   6.2892   23.412   1.8190   1.0000   1.0000
T, DEG K             338.9   1114.2    391.4    751.2   2575.2   1535.6   1348.0    298.1
RHO, G/CC         4.4854-4 1.2516-4 3.8631-4 2.9603-3 2.9603-3 3.8631-4 2.4194-4 1.4056-3
H, CAL/G           -134.85  -435.35  -152.78  -50.425   89.648  -293.90  -357.88  -806.15
U, CAL/G           -157.94  -518.08  -179.58  -101.88  -101.88  -407.93  -457.98  -823.38
S, CAL/(G)(K)       1.7473   2.2299   1.8020   1.8020   2.2299   2.2299   2.2299   1.4880
CP, CAL/(G)(K)      0.2600   0.3250   0.2657   0.3031   0.4223   0.3515   0.3370   0.9216
GAMMA (S)           1.3551   1.2961   1.3472   1.2919   1.2263   1.2679   1.2826   1.1406
M, MOL WT           29.170   26.763   29.015   29.015   26.719   26.762   26.762   34.389

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR                 0.00086  0.00790  0.00132  0.00132  0.00788  0.00790  0.00790  0.00790
C(S)               0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.04667
CH4                0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00005
CO                 0.00592  0.05434  0.00905  0.00905  0.06736  0.05437  0.05437  0.00000
CO2                0.00872  0.07996  0.01332  0.01332  0.06674  0.07995  0.07995  0.08764
H                  0.00000  0.00000  0.00000  0.00000  0.00117  0.00000  0.00000  0.00000
H2                 0.00433  0.03972  0.00662  0.00662  0.02715  0.03975  0.03975  0.00000
H2O(L)             0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.17480
H2O                0.01736  0.15927  0.02654  0.02654  0.17010  0.15925  0.15925  0.02419
NO                 0.00007  0.00060  0.00010  0.00010  0.00060  0.00060  0.00060  0.00000
N2                 0.07174  0.65821  0.10966  0.10966  0.65713  0.65818  0.65818  0.65875
O                  0.00000  0.00000  0.00000  0.00000  0.00005  0.00000  0.00000  0.00000
OH                 0.00000  0.00000  0.00000  0.00000  0.00169  0.00000  0.00000  0.00000
O2                 0.00000  0.00000  0.00000  0.00000  0.00012  0.00000  0.00000  0.00000
C3H8               0.04383  0.00000  0.04100  0.04100  0.00000  0.00000  0.00000  0.00000
AIR                0.84717  0.00000  0.79239  0.79239  0.00000  0.00000  0.00000  0.00000


TOTAL COMPUTER TIME=   2.164 SEC        DELTA TIME =  0.274 SEC
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```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   2    LEVEL 2    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.100      T(EGR) =  909.4 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM      ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN =  29.21 DEG     IVSHUT = 180.00 DEG                             EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =    3.200

                                                                          WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                              CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                             1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  *1.000000    -1386.340  G     298.15
                    * AIR INCLUDES   0.02348 MOLE FRACTION WATER           RELATIVE HUMIDITY= 0.7500

                  A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                    MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.49708                         CHARGE       13.2343                     EXHAUST      13.1828
     FUEL           0.03007                         FUEL          0.8769                     CO           0.48846
     AIR            0.37831                         AIR          11.0339                     NOX          0.00000

   ENERGY PER CYCLE (JOULES)                  AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK           390.663           INDICATED POWER          11.394                NET WORK       0.263839
 INDICATED PUMP WORK      -54.354           INDICATED PUMP POWER     -1.585                HEAT LOSS      0.282482
 HEAT LOSS                360.072           HEAT LOSS RATE           10.502                EXHAUST        0.465758
 CHEM. ENERGY            1274.674           EXHAUST POWER            17.316

                                                        MISCELLANEOUS

                                 INDICATED MEAN EFFECTIVE PRESSURE (ATM)                3.9907
                                 PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -0.5552
                                 MEAN TORQUE (NEWTON-METERS)                           26.7626

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  875.35 K   AND  1.0000 ATM      MOLECULAR WEIGHT =  26.770
     AR        0.007900       CO         0.035412       CO2        0.098946      H2         0.058132      H2O       0.140928
     NH3       0.000007       N2         0.658674

FRESH CHARGE MOLE FRACTIONS AT  293.79 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.171
     AR        0.000861       CO         0.004038       CO2        0.010603      H2         0.006156      H2O       0.015536
     N2        0.071776       C3H8       0.043835       AIR        0.847194

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   7.411 SEC
```

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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  11    LEVEL 5    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.100     T(EGR) =  900.6 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =   3.200

                                                                          WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                               CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                             1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  *1.000000    -1386.340  G    298.15
                  * AIR INCLUDES   0.02348 MOLE FRACTION WATER            RELATIVE HUMIDITY= 0.7500

                A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                     PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.49685                     CHARGE       12.6027                      EXHAUST       13.2527
     FUEL          0.02860                     FUEL          0.8351                      CO            0.71753
     AIR           0.35987                     AIR          10.5073                      NOX           0.00013
                                               NET          12.6376                      NET           13.2526

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK          404.672          INDICATED POWER          11.803           NET WORK      0.243361
 INDICATED PUMP WORK     -86.886          INDICATED PUMP POWER     -2.534           HEAT LOSS     0.269577
 HEAT LOSS               352.020          HEAT LOSS RATE           10.267           EXHAUST       0.435675
 CHEM. ENERGY           1305.823          EXHAUST POWER            16.593

                                                  MISCELLANEOUS

                             INDICATED MEAN EFFECTIVE PRESSURE (ATM)               4.1338
                             PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -0.8876
                             MEAN TORQUE (NEWTON-METERS)                          25.2886

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  900.63 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  26.947
     AR         0.007952       CH4        0.000914       CO         0.052088       CO2        0.077497       C2H2       0.002239
     C2H4       0.000131       H2         0.026569       H2O        0.169476       NO         0.000009       N2         0.663041
     O2         0.000070

FRESH CHARGE MOLE FRACTIONS AT  292.50 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.192
     AR         0.000861       CH4        0.000099       CO         0.005643       CO2        0.008395       C2H2       0.000243
     C2H4       0.000014       H2         0.002878       H2O        0.018359       N2         0.071827       O2         0.000008
     C3H8       0.043867       AIR        0.847803

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  48.858 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE  12    LEVEL 5    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100      T(EGR) =   901.9 K      SPARK ADVANCE =   20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =   966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                 EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00    C3 =      0.000000    A =  0.4000     B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE    COMBUSTION    TAU =0.8930E-04 SEC    BETA =    3.200
                                                                             WT FRACTION    ENERGY    STATE    TEMP
             CHEMICAL FORMULA                                                                CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                               1.000000    -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                    *1.000000     -1386.340  G     298.15
                    * AIR INCLUDES   0.02348 MOLE FRACTION WATER              RELATIVE HUMIDITY= 0.7500

                  A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.44855                      CHARGE        11.2684                      EXHAUST       12.6838
     FUEL           0.02555                      FUEL           0.7467                      CO            0.68590
     AIR            0.32149                      AIR            9.3949                      NOX           0.00012
                                                 NET           11.2425                      NET           12.6837

    ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

  INDICATED WORK          -14.459           INDICATED POWER          -0.422             NET WORK     -0.107273
  INDICATED PUMP WORK   -103.441            INDICATED PUMP POWER     -3.017             HEAT LOSS     0.054072
  HEAT LOSS               59.428            HEAT LOSS RATE            1.733             EXHAUST       0.496113
  CHEM. ENERGY          1099.070            EXHAUST POWER            15.903
                                                    MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)             -0.1477
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -1.0567
                               MEAN TORQUE (NEWTON-METERS)                         -9.3822

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT   901.89 K   AND   1.0000 ATM      MOLECULAR WEIGHT =   26.950
    AR         0.007953      CH4        0.000914      CO        0.052029      CO2       0.077486      C2H2       0.002263
    C2H4       0.000147      H2         0.026451      H2O       0.169553      NO        0.000008      N2         0.663094
    O2         0.000087

FRESH CHARGE MOLE FRACTIONS AT  292.63 K  AND   0.4276 ATM      MOLECULAR WEIGHT =   29.192
    AR         0.000861      CH4        0.000099      CO        0.005636      CO2       0.008393      C2H2       0.000245
    C2H4       0.000016      H2         0.002865      H2O       0.018366      N2        0.071828      O2         0.000009
    C3H8       0.043867      AIR        0.847810

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  66.090 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE  13    LEVEL 5    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.100     T(EGR) =  511.9 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                          EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000    C2 = 0.387200E 00    C3 =      0.000000     A =  0.4000     B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =   3.200

                                                                        WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                              CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                           1.000000    -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936    C  0.00032               *1.000000     -1386.340  G     298.15
                  * AIR INCLUDES   0.02348 MOLE FRACTION WATER          RELATIVE HUMIDITY= 0.7500

                A/F= 12.5823    PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                        PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46733                    CHARGE        9.4892                      EXHAUST      14.0309
     FUEL           0.02150                    FUEL          0.6288                      CO           0.33613
     AIR            0.27046                    AIR           7.9115                      NOX          0.00006
                                               NET           9.4717                      NET           8.9404

    ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

  INDICATED WORK          -13.881         INDICATED POWER         -0.405          NET WORK      -0.104220
  INDICATED PUMP WORK   -107.919          INDICATED PUMP POWER    -3.148          HEAT LOSS      0.034157
  HEAT LOSS               39.918          HEAT LOSS RATE           1.164          EXHAUST        0.885673
  CHEM. ENERGY          1168.676          EXHAUST POWER           30.189

                                                 MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)             -0.1418
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -1.1024
                              MEAN TORQUE (NEWTON-METERS)                         -9.6925

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  511.85 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.295
     AR         0.008350      CH4        0.000426      CO         0.024200      CO2        0.036184      C2H2       0.001051
     C2H4       0.000069      C3H8       0.026319      H2         0.012306      H2O        0.090780      N2         0.696205
     O2         0.104098

FRESH CHARGE MOLE FRACTIONS AT  255.81 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.344
     AR         0.000866      CH4        0.000044      CO         0.002510      CO2        0.003752      C2H2       0.000109
     C2H4       0.000007      C3H8       0.002729      H2         0.001276      H2O        0.009414      N2         0.072200
     O2         0.010796      C3H8       0.044094      AIR        0.852200

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  60.194 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                        CYCLE  14    LEVEL 5    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.100     T(EGR) =  418.8 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                              EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =   3.200

                                                                          WT FRACTION   ENERGY   STATE   TEMP
        CHEMICAL FORMULA                                                                CAL/MOL          DEG K
FUEL     C  3.00000   H  8.00000                                            1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936    C  0.00032                *1.000000    -1386.340  G     298.15
                   * AIR INCLUDES   0.02348 MOLE FRACTION WATER           RELATIVE HUMIDITY= 0.7500

                A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.51834                     CHARGE        9.3578                     EXHAUST      15.9305
     FUEL          0.02116                     FUEL          0.6201                     CO           0.25360
     AIR           0.26621                     AIR           7.8020                     NOX          0.00005
                                               NET           9.3652                     NET           7.8639

    ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK          430.817          INDICATED POWER         12.565              NET WORK       0.254045
 INDICATED PUMP WORK     -80.372          INDICATED PUMP POWER    -2.344              HEAT LOSS      0.262173
 HEAT LOSS               361.657          HEAT LOSS RATE          10.548              EXHAUST        0.955630
 CHEM. ENERGY           1379.461          EXHAUST POWER           38.449

                                                 MISCELLANEOUS

                                 INDICATED MEAN EFFECTIVE PRESSURE (ATM)              4.4009
                                 PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8210
                                 MEAN TORQUE (NEWTON-METERS)                         27.8875

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  418.78 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.677
     AR        0.008463     CH4       0.000288      CO        0.016298     CO2       0.024455     C2H2      0.000708
     C2H4      0.000047     C3H8      0.033790      H2        0.008285     H2O       0.068419     N2        0.705606
     O2        0.133630

FRESH CHARGE MOLE FRACTIONS AT  247.61 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.384
     AR        0.000867     CH4       0.000029      CO        0.001670     CO2       0.002506     C2H2      0.000073
     C3H8      0.003462     H2        0.000849      H2O       0.007011     N2        0.072300     O2        0.013692
     C3H8      0.044155     AIR       0.853379

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  47.411 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  15    LEVEL 5    CASE NO.      111
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.100      T(EGR) =  904.2 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                 EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =   3.200

                                                                          WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                               CAL/MOL            DEG K
FUEL    C  3.00000   H  8.00000                                              1.000000   -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                    *1.000000    -1386.340  G     298.15
                  * AIR INCLUDES   0.02348 MOLE FRACTION WATER             RELATIVE HUMIDITY= 0.7500

                     A/F= 12.5823   PERCENT FUEL=   7.3625   EQUIVALENCE RATIO= 1.2500   PHI=   1.2647

                                        PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.49664                     CHARGE        12.6031                      EXHAUST        13.3150
     FUEL           0.02862                     FUEL           0.8351                      CO              0.72181
     AIR            0.36009                     AIR           10.5077                      NOX             0.00013
                                                NET           12.6390                      NET            13.3149

   ENERGY PER CYCLE (JOULES)               AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK          404.608           INDICATED POWER         11.801              NET WORK       0.243227
 INDICATED PUMP WORK     -86.883           INDICATED PUMP POWER    -2.534              HEAT LOSS      0.269524
 HEAT LOSS               352.076           HEAT LOSS RATE          10.269              EXHAUST        0.439217
 CHEM. ENERGY           1306.290           EXHAUST POWER           16.734
                                                        MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              4.1332
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8875
                              MEAN TORQUE (NEWTON-METERS)                         25.2837

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT  904.20 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  26.946
     AR        0.007952      CH4       0.000905      CO       0.052151      CO2       0.077467      C2H2       0.002217
     C2H4      0.000138      H2        0.026606      H2O      0.169458      NO        0.000009      N2         0.663013
     O2        0.000070

FRESH CHARGE MOLE FRACTIONS AT  292.86 K  AND  0.4276 ATM       MOLECULAR WEIGHT =  29.192
     AR        0.000861      CH4       0.000098      CO       0.005650      CO2       0.008392      C2H2       0.000240
     C2H4      0.000015      H2        0.002882      H2O      0.018358      N2        0.071827      O2         0.000008
     C3H8      0.043867      AIR       0.847799

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  56.502 SEC
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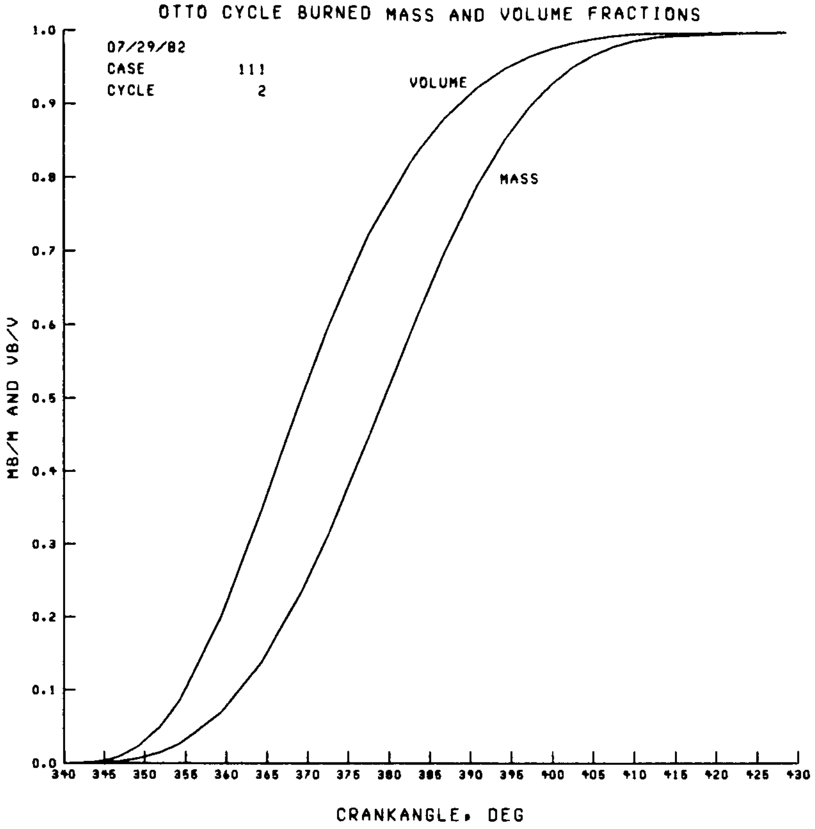
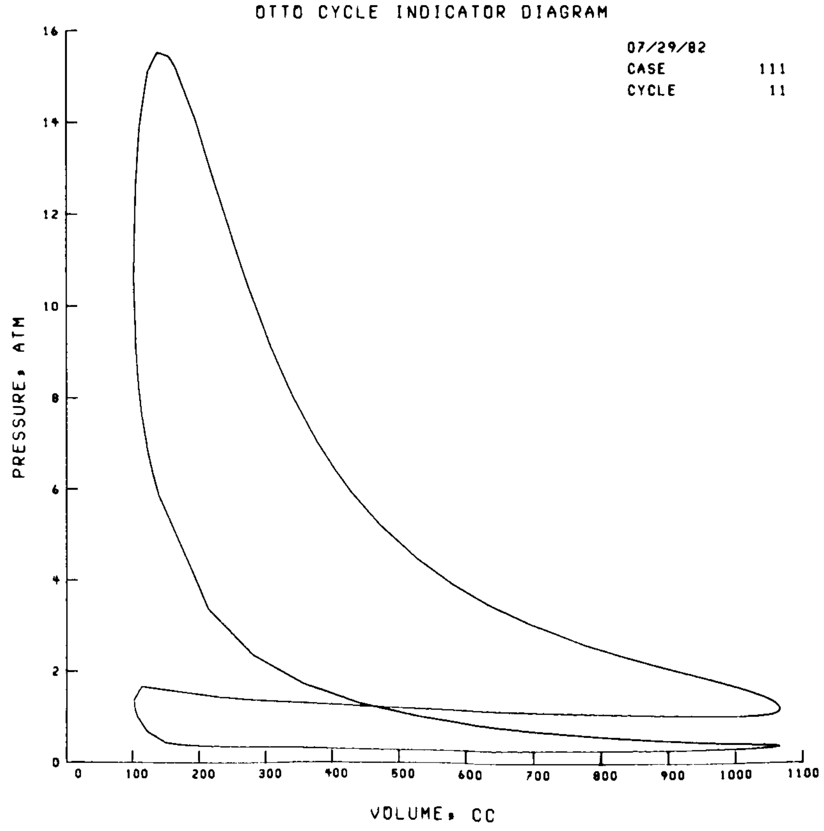
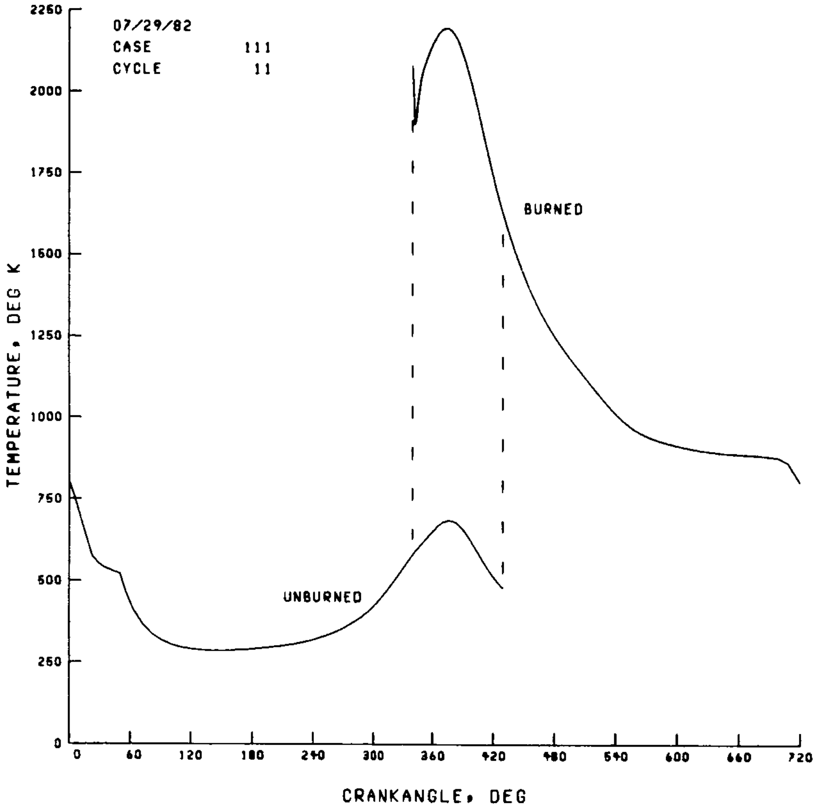
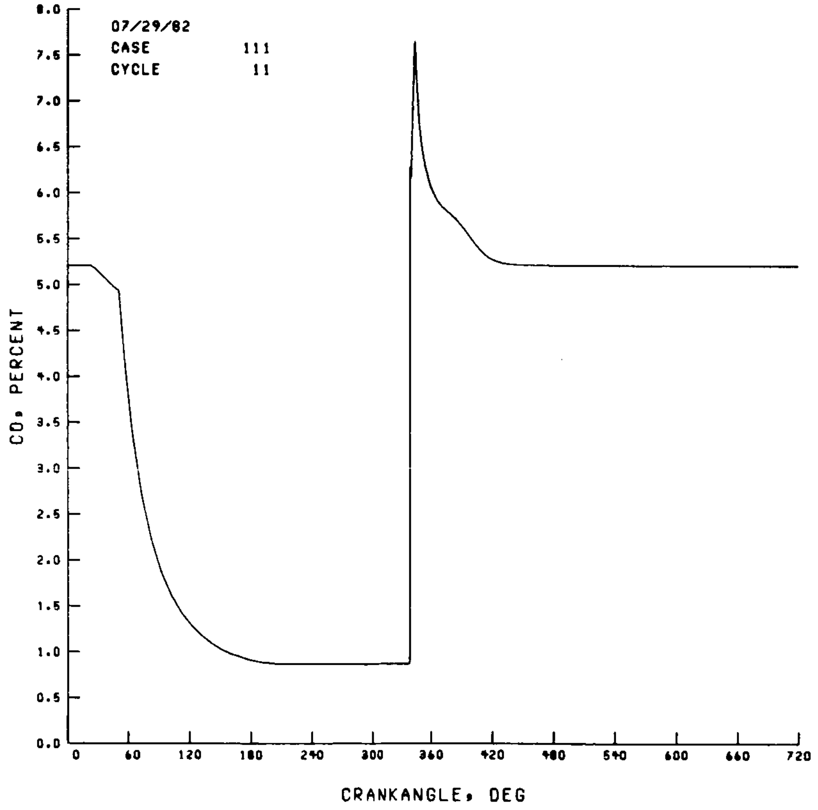
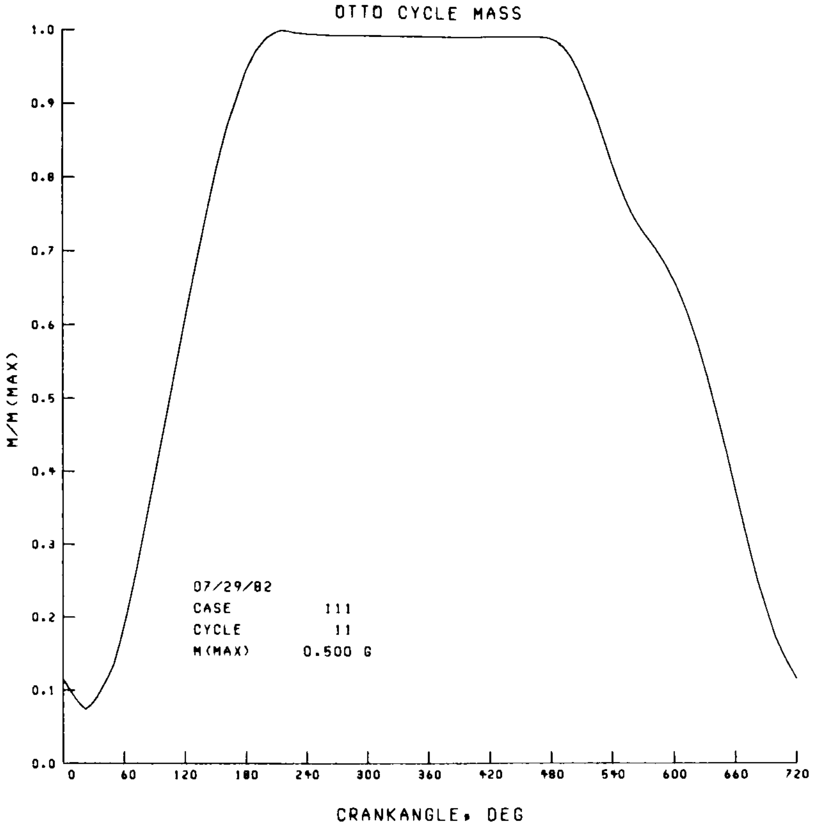
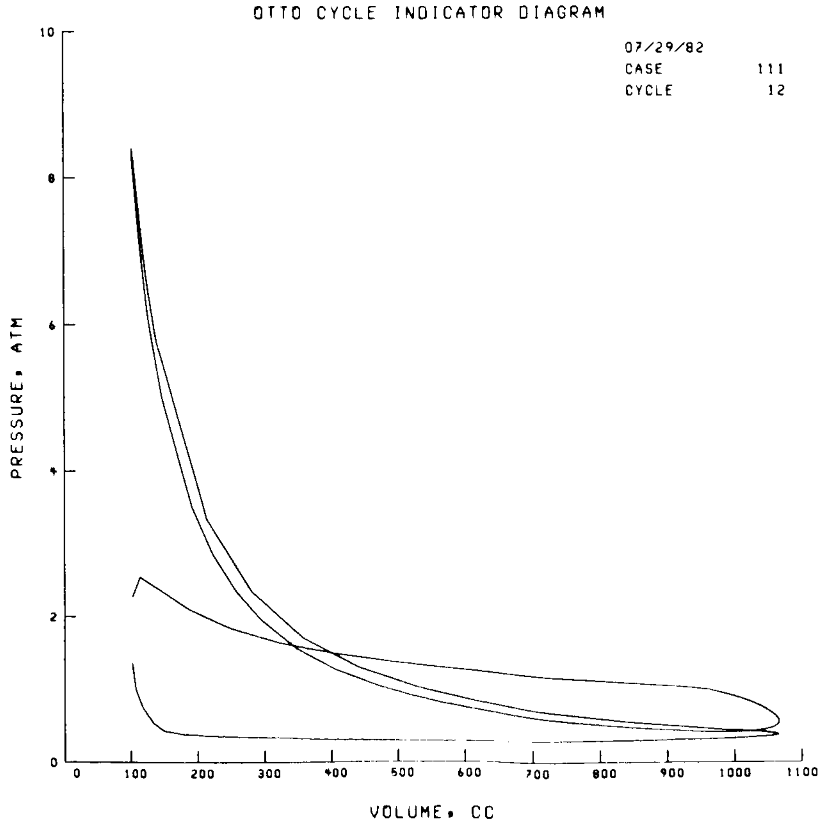

OTTO CYCLE BURNED MASS AND VOLUME FRACTIONS
07/29/82
CASE 111
CYCLE 2
VOLUME
MASS
MB/M AND VB/V
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
340
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
425
430
CRANKANGLE, DEG

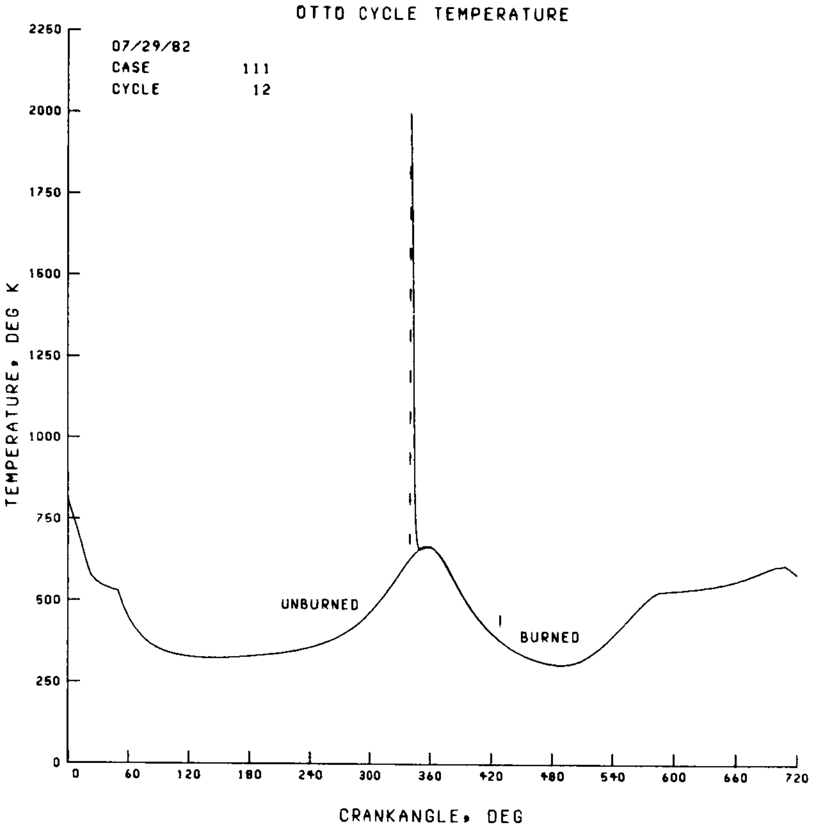

OTTO CYCLE INDICATOR DIAGRAM
07/29/82
CASE 111
CYCLE 11
PRESSURE, ATM
16
14
12
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
1000
1100
VOLUME, CC

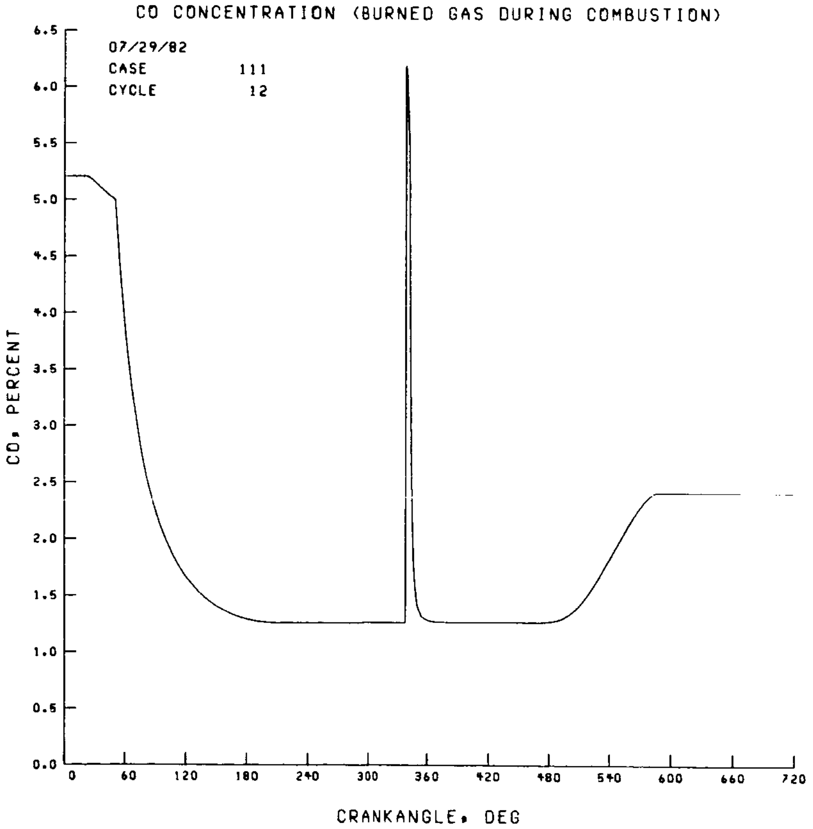

OTTO CYCLE TEMPERATURE

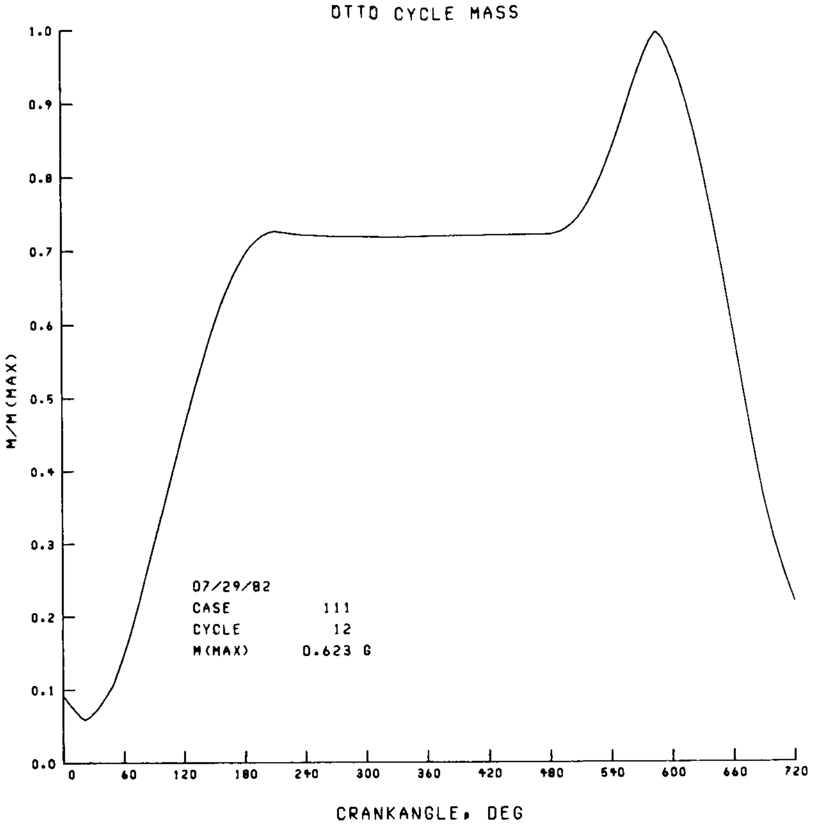

CO CONCENTRATION (BURNED GAS DURING COMBUSTION)

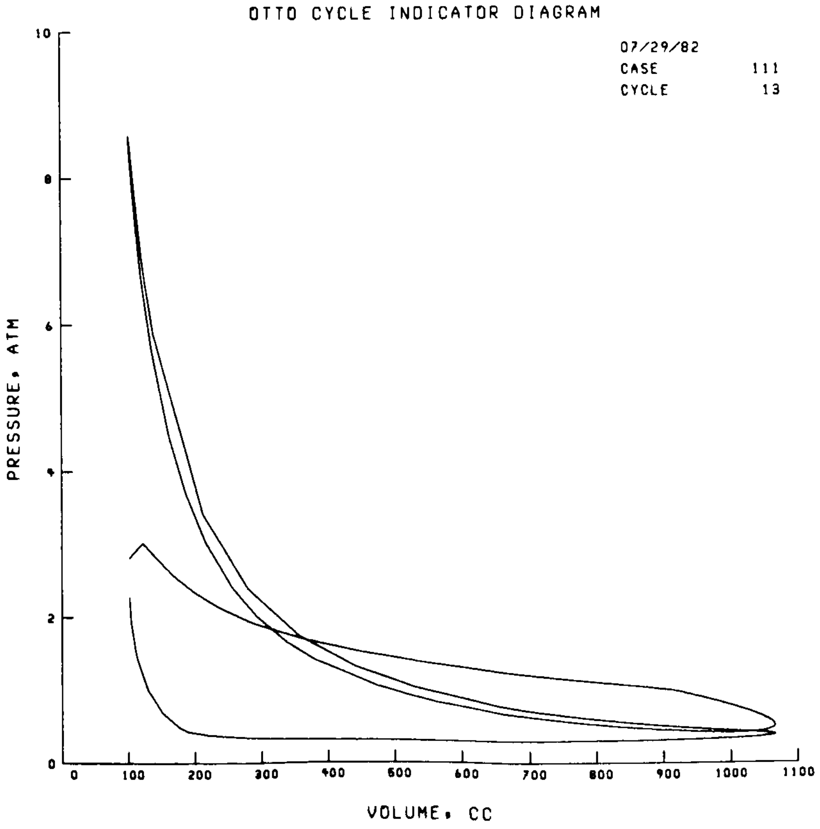

OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG
07/29/82
CASE 111
CYCLE 11
M(MAX) 0.500 G

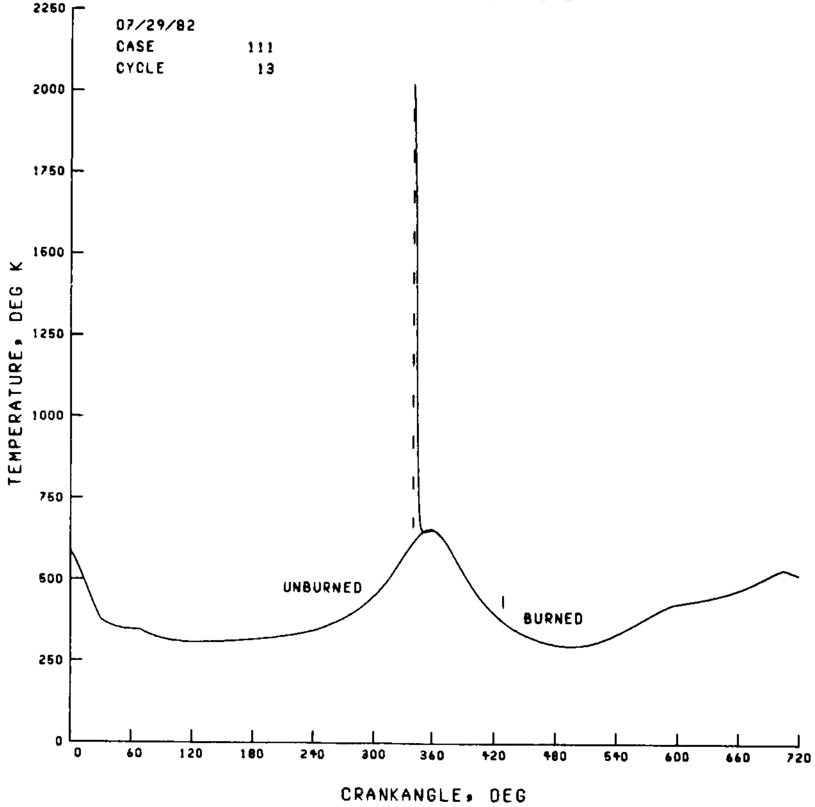

OTTO CYCLE INDICATOR DIAGRAM
07/29/82
CASE 111
CYCLE 12
PRESSURE, ATM
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
1000
1100
VOLUME, CC


OTTO CYCLE TEMPERATURE

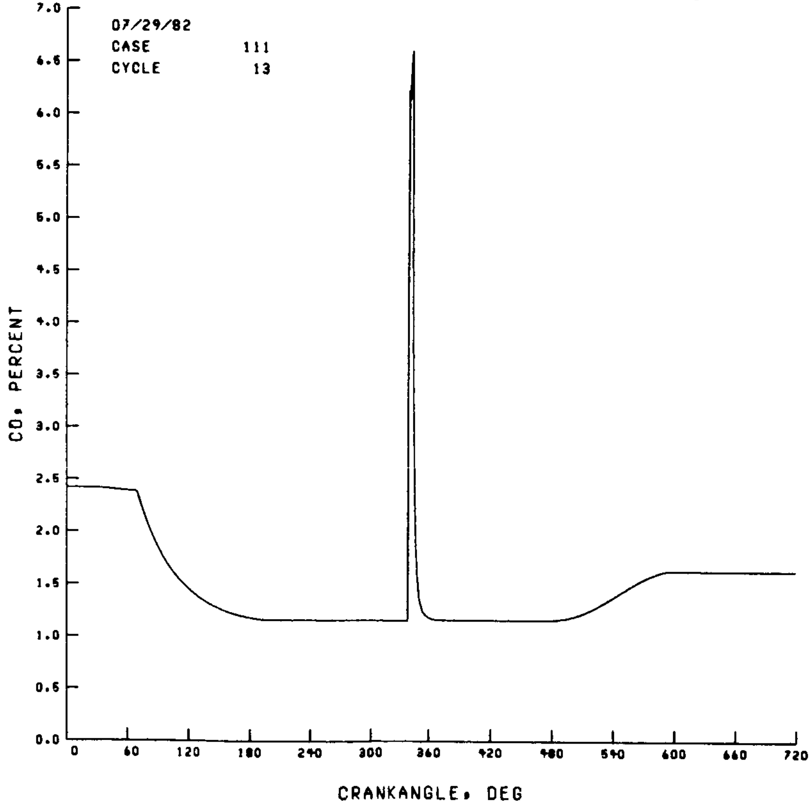

CO CONCENTRATION (BURNED GAS DURING COMBUSTION)


OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
07/29/82
CASE 111
CYCLE 12
M(MAX) 0.623 G
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

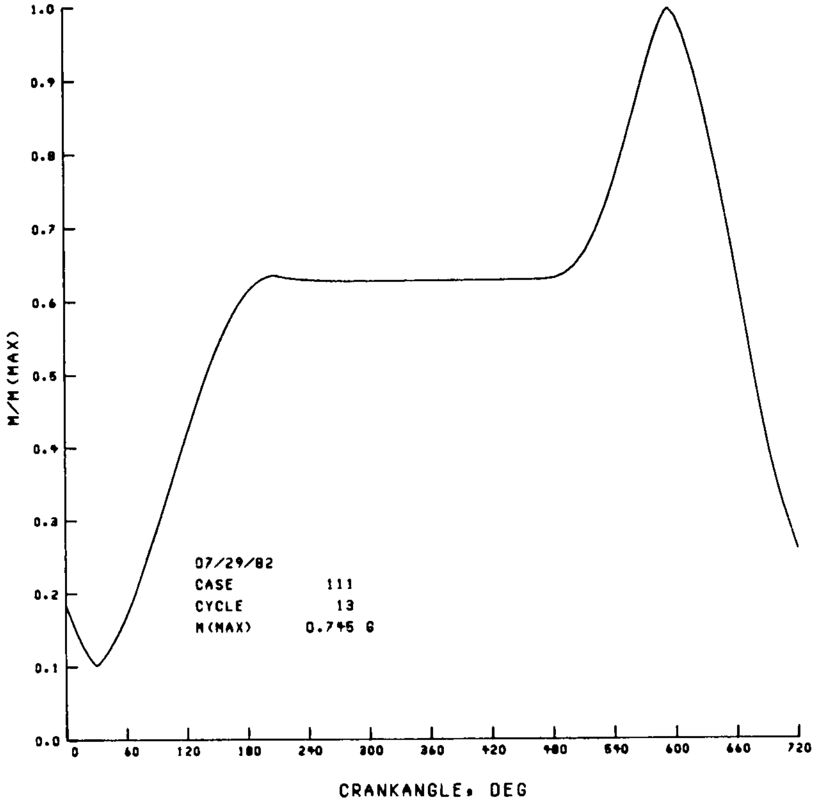

OTTO CYCLE INDICATOR DIAGRAM
07/29/82
CASE 111
CYCLE 13
PRESSURE, ATM
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
1000
1100
VOLUME, CC



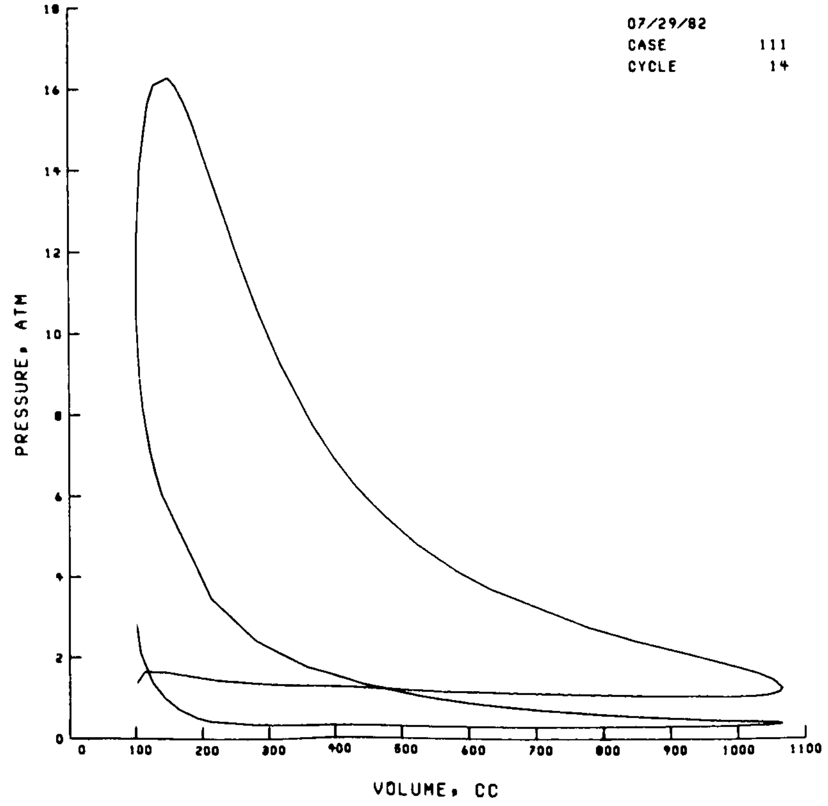
OTTO CYCLE TEMPERATURE



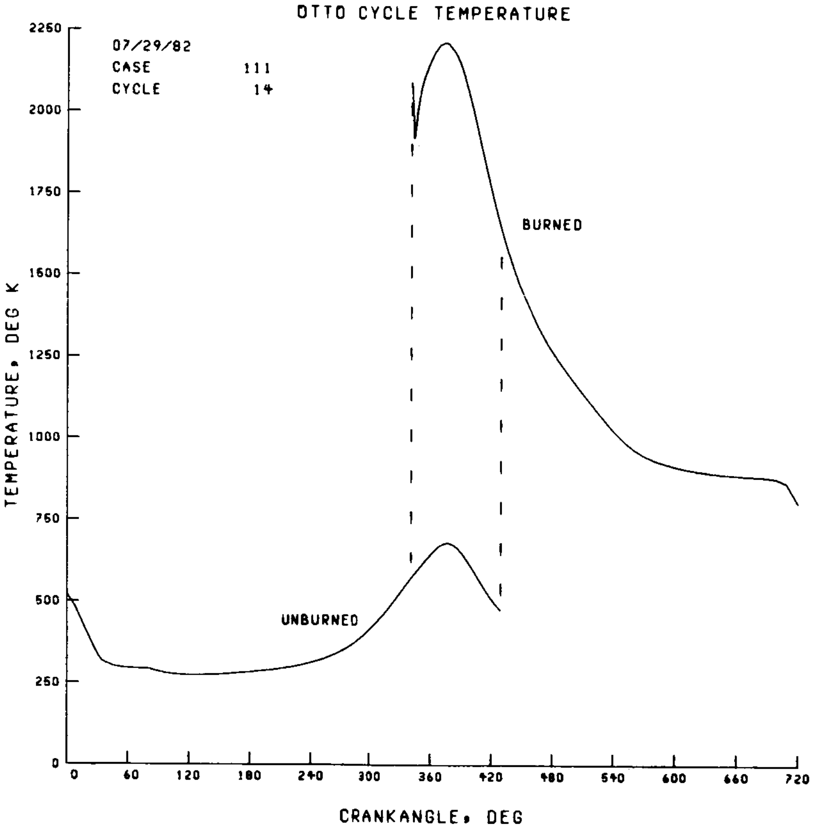
CO CONCENTRATION (BURNED GAS DURING COMBUSTION)

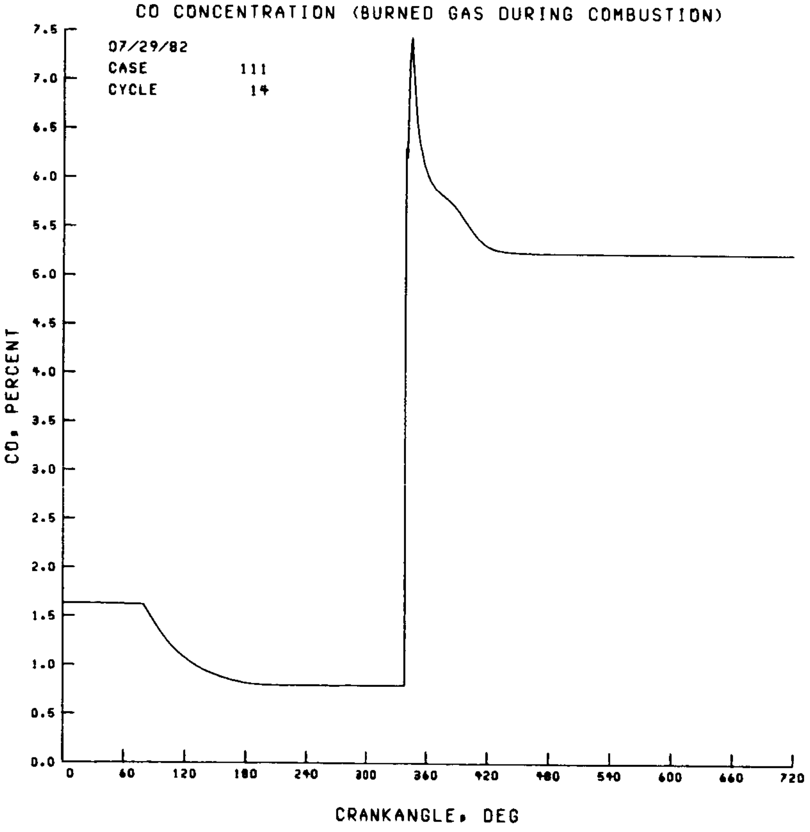


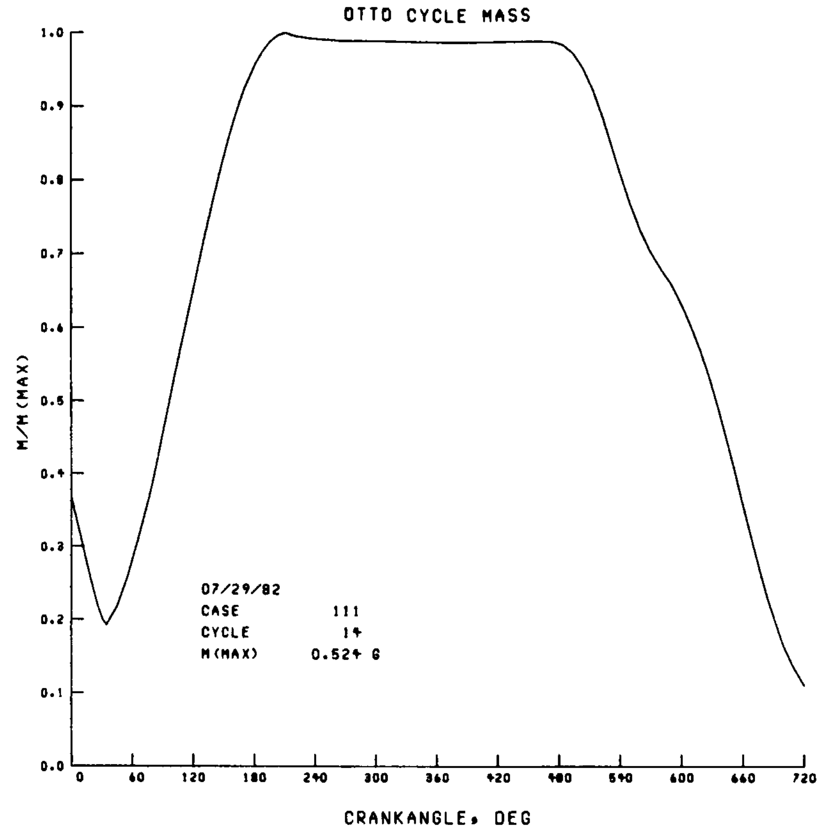
OTTO CYCLE MASS

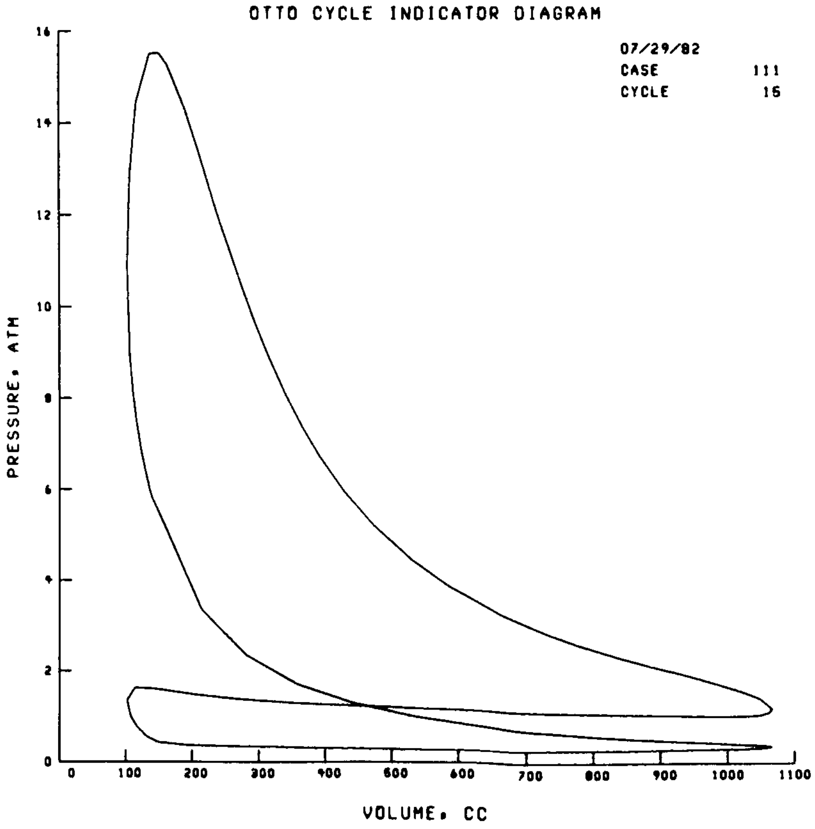


OTTO CYCLE INDICATOR DIAGRAM

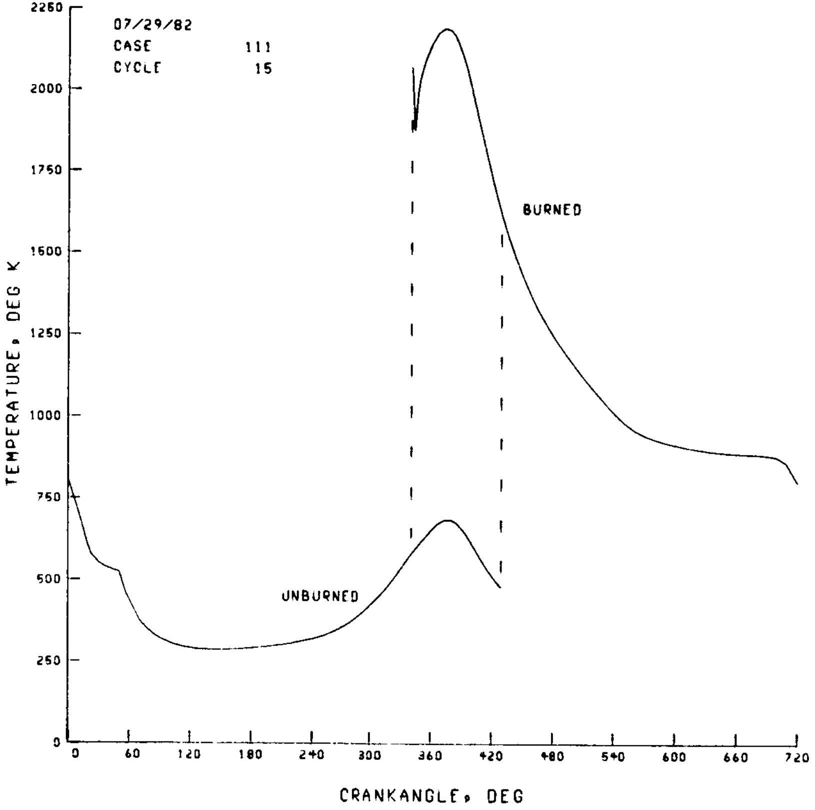

OTTO CYCLE TEMPERATURE
07/29/82
CASE 111
CYCLE 14
BURNED
UNBURNED
TEMPERATURE, DEG K
2250
2000
1750
1500
1250
1000
750
500
250
0
CRANKANGLE, DEG
0
60
120
180
240
300
360
420
480
540
600
660
720


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 111
CYCLE 14
CO, PERCENT
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
CRANKANGLE, DEG
0
60
120
180
240
300
360
420
480
540
600
660
720

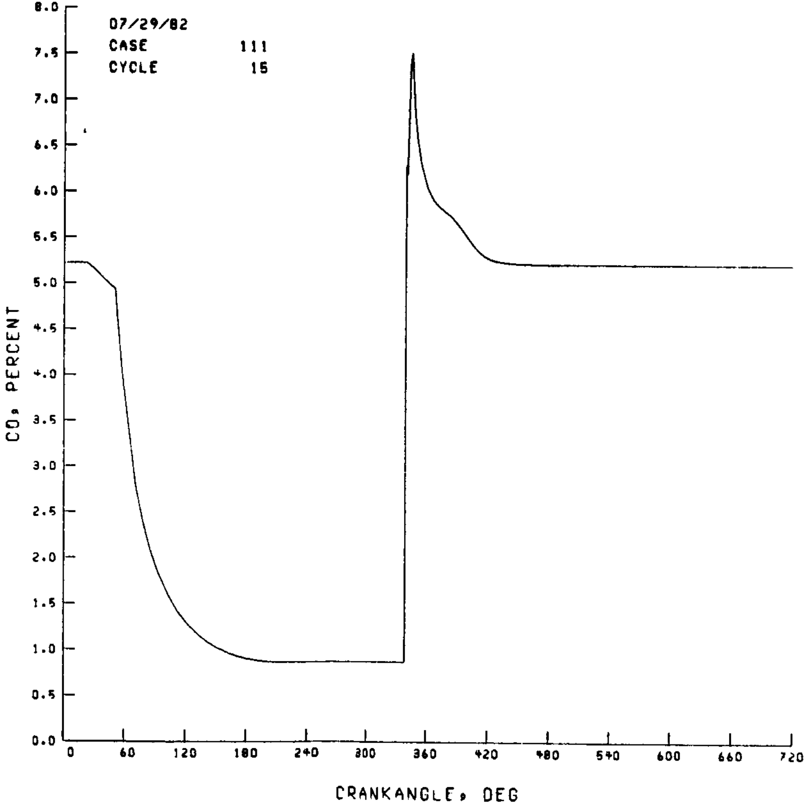

OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG
07/29/82
CASE 111
CYCLE 14
M(MAX) 0.524 G

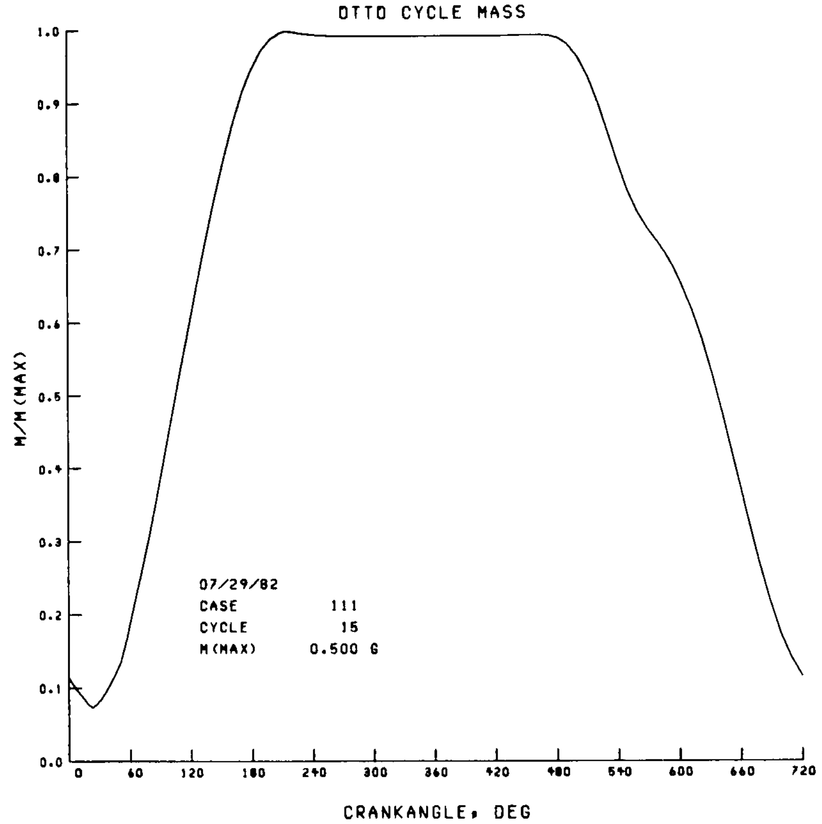

OTTO CYCLE INDICATOR DIAGRAM
07/29/82
CASE 111
CYCLE 15
PRESSURE, ATM
16
14
12
10
8
6
4
2
0
0
100
200
300
400
500
600
700
800
900
1000
1100
VOLUME, CC

OTTO CYCLE TEMPERATURE



CO CONCENTRATION (BURNED GAS DURING COMBUSTION)




OTTO CYCLE MASS
M/M(MAX)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG
07/29/82
CASE 111
CYCLE 15
M(MAX) 0.500 G

Appendix H

Example V (Case 10)

Input, Case 10

```
REAC
N 1.     H 3.                                2.     M         G  298.15
N 2.                                         5.59138M         G 298.15
O 2.                                         1.5    M         G 298.15
AR1.                                         .067060M         G 298.15
C 1.     O 2.                                .002284M         G 298.15

NAME
 &OTTINP FREQ=3500,BORE=10.922,STROKE=10.312,ROD=17.145,CA=129.03,
 TW=360.,CR=10.5,BETA=3.2,KASE=10,TRACE=1.E-20,
 PEXH=1.,PMFOLD=.4276,
 &END
 &AFINP DEBUG=T,AF=.00001,SPARK=20.,THBURN=110.,
 NCYCLE=5,TAU=8.93E-05,VARAF=F&END
```

Output, Case 10

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   5    LEVEL 1    CASE NO.        10
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM    MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                              MOLES       ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                  CAL/MOL          DEG K
FUEL    N  1.00000   H  3.00000                                                2.000000   -10970.801  G    298.10
FUEL    N  2.00000                                                             5.591379        0.000  G    298.15
FUEL    O  2.00000                                                             1.500000        0.000  G    298.15
FUEL    AR 1.00000                                                             0.067060        0.000  G    298.15
FUEL    C  1.00000   O  2.00000                                                0.002284   -94049.563  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F=  0.0000   PERCENT FUEL=  99.9990   EQUIVALENCE RATIO= 1.0000   PHI=   0.0000
FUEL MASS FRACTION = 0.953854                       INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  6.0311
AIR MASS FRACTION = 0.000010                        PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.5513
RESIDUAL MASS FRACTION = 0.046137                   CHEMICAL ENERGY (JOULES/G) =3012.758
RECIRCULATED MASS FRACTION = 0.000000               MASS EFFICIENCY = 0.953863
MASS FRACTION EXHAUST RETAINED = 0.046137           VOLUME EFFICIENCY = 0.816515
NET WORK EFFICIENCY = 0.339326                      FRACTIONAL MASS CHANGE 6 - 7 =-0.515558

THERMODYNAMIC PROPERTIES

STATION                          2        3        4        5        6        7
CRANKANGLE       0.0000   32.054   180.00   340.00   340.00   540.00   540.00   0.0000
P, ATM           0.4276   0.4276   0.4276   6.7911   31.888   2.5283   1.0000   1.0000
T, DEG K          236.2   1052.8    278.8    577.9   2564.0   1565.2   1277.9    298.1
RHO, G/CC      5.8157-4 1.2356-4 4.9140-4 3.7655-3 3.7655-3 4.9140-4 2.3805-4 1.4359-3
H, CAL/G        -108.79  -474.35  -125.66  -39.418   121.99  -291.05  -395.73  -840.37
U, CAL/G        -126.60  -558.16  -146.73  -83.093  -83.094  -415.65  -497.46  -857.23
S, CAL/(G)(K)    1.8293   2.3331   1.8919   1.8919   2.3331   2.3331   2.3331   1.5039
CP, CAL/(G)(K)   0.2737   0.3415   0.2764   0.3030   0.5129   0.3719   0.3564   0.9767
GAMMA (S)        1.3802   1.3040   1.3764   1.3323   1.2058   1.2724   1.2876   1.1241
M, MOL WT        26.359   24.963   26.292   26.292   24.844   24.963   24.963   35.130

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR             0.0000 0 6.9326-3 3.3687-4 3.3687-4 6.8996-3 6.9326-3 6.9326-3 6.9415-3
CH4            0.000  0 3.898-18 1.894-19 1.894-19 2.202-16 3.940-18 3.940-18 0.000  0
CO             0.0000 0 5.4763-6 2.6611-7 2.6611-7 3.7489-5 5.4903-6 5.4903-6 0.0000 0
CO2            0.0000 0 2.3064-4 1.1208-5 1.1208-5 1.9751-4 2.3063-4 2.3063-4 2.3642-4
H              0.0000 0 1.1817-6 5.7420-8 5.7420-8 5.5143-4 1.1831-6 1.1831-6 0.0000 0
HO2            0.000  0 2.884-11 1.402-12 1.402-12 3.769 -6 2.872-11 2.872-11 0.000  0
H2             0.0000 0 2.5648-3 1.2463-4 1.2463-4 8.9652-3 2.5716-3 2.5716-3 0.0000 0
H2O(L)         0.0000 0 0.0000 0 0.0000 0 0.0000 0 0.0000 0 0.0000 0 0.0000 0 2.8850-1
H2O            0.0000 0 3.0756-1 1.4945-2 1.4945-2 2.9733-1 3.0756-1 3.0756-1 2.2037-2
NH3            0.000  0 1.426 -8 6.927-10 6.927-10 2.274 -7 1.431 -8 1.431 -8 0.000  0
N              0.000  0 1.547-13 7.515-15 7.515-15 7.527 -8 1.546-13 1.546-13 0.000  0
NO             0.0000 0 2.5796-3 1.2535-4 1.2535-4 2.5666-3 2.5789-3 2.5789-3 0.0000 0
NO2            0.000  0 5.678-12 2.759-13 2.759-13 1.129 -6 5.646-12 5.646-12 0.000  0
N2             0.0000 0 6.8012-1 3.3049-2 3.3049-2 6.7688-1 6.8012-1 6.8012-1 6.8229-1
O              0.000  0 1.936 -9 9.408-11 9.408-11 1.639 -4 1.931 -9 1.931 -9 0.000  0
OH             0.0000 0 5.1323-6 2.4939-7 2.4939-7 4.1640-3 5.1247-6 5.1247-6 0.0000 0
O2             0.0000 0 1.0672-7 5.1860-9 5.1860-9 2.2311-3 1.0613-7 1.0613-7 0.0000 0
AR             7.3203-3 0.0000 0 6.9646-3 6.9646-3 0.0000 0 0.0000 0 0.0000 0 0.0000 0
CO2            2.4932-4 0.0000 0 2.3721-4 2.3721-4 0.0000 0 0.0000 0 0.0000 0 0.0000 0
N2             6.1036-1 0.0000 0 5.8070-1 5.8070-1 0.0000 0 0.0000 0 0.0000 0 0.0000 0
O2             1.6374-1 0.0000 0 1.5578-1 1.5578-1 0.0000 0 0.0000 0 0.0000 0 0.0000 0
NH3            2.1832-1 0.0000 0 2.0771-1 2.0771-1 0.0000 0 0.0000 0 0.0000 0 0.0000 0
AIR            9.1003-6 0.0000 0 8.6581-6 8.6581-6 0.0000 0 0.0000 0 0.0000 0 0.0000 0


TOTAL COMPUTER TIME=   0.945 SEC         DELTA TIME =  0.151 SEC
```

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                   CYCLE   5    LEVEL 2    CASE NO.       10
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.000     T(EGR) =  298.1 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM    MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN =  30.29 DEG     IVSHUT = 180.00 DEG                          EVOPEN = 540.00 DEG     EVSHUT = 720.00 DEG

EICHELBERG HEAT TRANSFER COEFICIENT

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL = 88.7 DEG    WIEBE   COMBUSTION    TAU =0.8930E-04 SEC    BETA =   3.200

                                                                                      MOLES       ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                         CAL/MOL           DEG K
FUEL     N  1.00000   H  3.00000                                                   2.000000    -10970.801  G      298.10
FUEL     N  2.00000                                                                5.591379         0.000  G      298.15
FUEL     O  2.00000                                                                1.500000         0.000  G      298.15
FUEL     AR 1.00000                                                                0.067060         0.000  G      298.15
FUEL     C  1.00000   O  2.00000                                                   0.002284    -94049.563  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                         1.000000       -29.792  G      298.15

                  A/F=  0.0000   PERCENT FUEL=  99.9990   EQUIVALENCE RATIO= 1.0000   PHI=   0.0000

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.53867                         CHARGE        14.7819                      EXHAUST       14.7819
     FUEL          0.50681                         FUEL          14.7818                      CO            0.00000
     AIR           0.00001                         AIR            0.0001                      NOX           0.00291

   ENERGY PER CYCLE (JOULES)               AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

  INDICATED WORK          560.774         INDICATED POWER          16.356               NET WORK        0.315873
  INDICATED PUMP WORK     -54.205         INDICATED PUMP POWER     -1.581               HEAT LOSS       0.131208
  HEAT LOSS               210.420         HEAT LOSS RATE            6.137               EXHAUST         0.509798
  CHEM. ENERGY           1603.709         EXHAUST POWER            23.846

                                                         MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)           5.7284
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)               -0.5537
                              MEAN TORQUE (NEWTON-METERS)                      40.3115

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1091.06 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  24.993
     AR        0.006941      CO        0.000000     CO2       0.000236      H         0.000000     HO2        0.000000
     H2        0.000160      H2O       0.310347     NH3       0.000000      N         0.000000     NO         0.000164
     NO2       0.000000      N2        0.682150     O         0.000000      OH        0.000001     O2         0.000000

FRESH CHARGE MOLE FRACTIONS AT  236.19 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  26.359
     AR        0.007320      CO2       0.000249     N2        0.610358      O2        0.163741     NH3        0.218321
     AIR       0.000009

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   4.094 SEC
```

Appendix I

Example VI (Case 222)

Input, Case 222, Initial Run

```
REAC
C 3.     H 8.                                   1.               G298.15  F

NAME
 &OTTINP FREQ=3500,BORE=10.922,STROKE=10.312,ROD=17.145,CA=129.03,
 TW=360.,CR=10.5,AN=.375,-.5,.125,KASE=222,
 PEXH=1.,PMFOLD=.4276,
 HC3=0.,HA=.4,HB=.8,HC2=.3872,
   SP=T,TAIR=298.15&END
 &AFINP DEBUG=T,EQRAT=1.,SPARK=20.,EGR=.05,THBURN=110.,
 NCYCLE=10,IFLOW=4,VARAF=F,KFLAME=4&END
 &FLOWIN DIN=4.78155,DEX=3.65125,BETAIN=45,BETAEX=45,LIN=2.2,LINR=2.2,
  LEX=1.8,LEXR=1.8,AIN(1)=.95,AINR(1)=1.,AEXR(1)=.95,
  EIN(2)=-20,EINR(2)=-20,EEXR(2)=-15,EEX(2)=-15,EIN(3)=2,EINR(3)=2,
  EEXR(3)=2,EEX(3)=2,BIN(1)=.05,BINR(1)=.05,AEX(1)=1.,
  RIN=.11655397536916,-1.2305226637252,53.276925905521,-329.46664003586,967.59957726191,
  -1606.5917666613,1531.2782499752,-777.72614964883,162.74377189163,
  REX=.015239819814648,1.2692256549564,24.316014460188,-83.715719936202,
  -146.81709604486,1257.7189438064,-2839.5867388125,3151.0342473402,
  -1758.248769365,394.01465307699,POLY=T,
  IVOPEN=699,IVSHUT=265,EVOPEN=465,EVSHUT=45&END
```

Input, Case 222, First Restart

```
RESTART
 &AFINP  VARAF=T,AF= 13.074351&END
 &AFINP  VARAF=T,AF= 13.464056&END
 &AFINP  VARAF=T,AF= 13.876776&END
 &AFINP  VARAF=T,AF= 12.629932&END
 &AFINP  VARAF=T,AF= 13.958652&END
 &AFINP  VARAF=T,AF= 14.866378&END
 &AFINP  VARAF=T,AF= 16.708862&END
 &AFINP  VARAF=T,AF= 19.213028&END
 &AFINP  VARAF=T,AF= 18.456665&END
 &AFINP  VARAF=F,AF= 16.368179&END
```

Input, Case 222, Second Restart

```
RESTART 21
 &AFINP  VARAF=T,AF= 14.914374&END
 &AFINP  VARAF=T,AF= 16.414169&END
 &AFINP  VARAF=T,AF= 17.009354&END
 &AFINP  VARAF=T,AF= 14.286650&END
 &AFINP  VARAF=T,AF= 16.018585&END
 &AFINP  VARAF=T,AF= 12.948669&END
 &AFINP  VARAF=T,AF= 13.566860&END
 &AFINP  VARAF=T,AF= 16.184128&END
 &AFINP  VARAF=T,AF= 15.951797&END
 &AFINP  VARAF=F,AF= 14.974538&END
```

Input, Case 222, Third Restart

```
RESTART 31
 &AFINP  VARAF=T,AF=  14.289288&END
 &AFINP  VARAF=T,AF=  15.469439&END
 &AFINP  VARAF=T,AF=  12.718887&END
 &AFINP  VARAF=T,AF=  16.008972&END
 &AFINP  VARAF=T,AF=  14.313013&END
 &AFINP  VARAF=T,AF=  16.063583&END
 &AFINP  VARAF=F,AF=  19.820328&END
```

Output, Case 222

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                     CYCLE   5    LEVEL 1    CASE NO.     222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.050      T(EGR) = 1483.3 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC

                                                                           WT FRACTION   ENERGY    STATE    TEMP
            CHEMICAL FORMULA                                                             CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                             1.000000   -24821.770  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                   1.000000      -29.792  G      298.15

                      A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000
FUEL MASS FRACTION = 0.054087                               INDICATED MEAN EFFECTIVE PRESSURE (ATM) =  5.0419
AIR MASS FRACTION = 0.848014                                PUMP MEAN EFFECTIVE PRESSURE (ATM) = -0.5509
RESIDUAL MASS FRACTION = 0.050420                           CHEMICAL ENERGY (JOULES/G) =2712.256
RECIRCULATED MASS FRACTION = 0.047479                       MASS EFFICIENCY = 0.949580
MASS FRACTION EXHAUST RETAINED = 0.050414                   VOLUME EFFICIENCY = 0.814630
NET WORK EFFICIENCY = 0.345119                              FRACTIONAL MASS CHANGE 6 - 7 =-0.470650

THERMODYNAMIC PROPERTIES


STATION                        2         3         4         5         6         7
CRANKANGLE        0.0000    32.406    180.00    340.00    340.00    540.00    540.00    0.0000
P, ATM            0.4276    0.4276    0.4276    6.4934    26.777    2.2365    1.0000    1.0000
T, DEG K           294.6    1234.5     348.9     691.4    2710.8    1756.2    1483.4     298.1
RHO, G/CC      5.2204-4 1.1963-4 4.3983-4 3.3704-3 3.3704-3 4.3983-4 2.3282-4 1.3319-3
H, CAL/G         -67.860   -408.70   -85.045    7.5171    153.26   -236.62   -327.86   -746.10
U, CAL/G         -87.696   -495.26   -108.59   -39.140   -39.140   -359.76   -431.87   -764.28
S, CAL/(G)(K)     1.6763    2.1518    1.7317    1.7317    2.1519    2.1519    2.1519    1.5334
CP, CAL/(G)(K)    0.2498    0.3190    0.2544    0.2868    0.5735    0.3407    0.3298    0.9192
GAMMA (S)         1.3690    1.2817    1.3610    1.3077    1.1768    1.2595    1.2700    1.1512
M, MOL WT         29.509    28.342    29.448    29.448    27.998    28.340    28.340    32.586

NOTES ON MOLE FRACTIONS:
A) STATION 2 RESIDUAL GAS FROM PREVIOUS CYCLE; B) MOLES NO FROZEN AFTER COMBUSTION(STATION 5)

MOLE FRACTIONS

AR                0.00045  0.00861  0.00088  0.00088  0.00851  0.00861  0.00861  0.00864
CO                0.00024  0.00452  0.00046  0.00046  0.02070  0.00458  0.00458  0.00000
CO2               0.00580  0.11135  0.01133  0.01133  0.09379  0.11132  0.11132  0.11626
H                 0.00000  0.00001  0.00000  0.00000  0.00079  0.00001  0.00001  0.00000
HO2               0.00000  0.00000  0.00000  0.00000  0.00001  0.00000  0.00000  0.00000
H2                0.00009  0.00171  0.00017  0.00017  0.00477  0.00173  0.00173  0.00000
H2O(L)            0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.12752
H2O               0.00793  0.15238  0.01550  0.01550  0.14396  0.15238  0.15238  0.02711
NO                0.00033  0.00629  0.00064  0.00064  0.00621  0.00629  0.00629  0.00000
N2                0.03723  0.71508  0.07274  0.07274  0.70640  0.71505  0.71505  0.72048
O                 0.00000  0.00000  0.00000  0.00000  0.00065  0.00000  0.00000  0.00000
OH                0.00000  0.00004  0.00000  0.00000  0.00627  0.00004  0.00004  0.00000
O2                0.00000  0.00000  0.00000  0.00000  0.00793  0.00000  0.00000  0.00000
C3H8              0.03812  0.00000  0.03612  0.03612  0.00000  0.00000  0.00000  0.00000
AIR               0.90982  0.00000  0.86216  0.86216  0.00000  0.00000  0.00000  0.00000


TOTAL COMPUTER TIME=   1.730 SEC         DELTA TIME =  0.224 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   3    LEVEL 2    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1208.7 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
PRESSURE DISCONTINUITIES ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN =  29.11 DEG      IVSHUT = 180.00 DEG                            EVOPEN = 540.00 DEG      EVSHUT = 720.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000     B =  0.8000

EQUILIBRIUM FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000


                                                                          WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                               CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                            1.000000   -24821.770  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  1.000000      -29.792  G      298.15

                  A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                       PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

    TOTAL         0.51657                       CHARGE       13.9806                     EXHAUST       13.9790
    FUEL          0.02730                       FUEL          0.7963                     CO             0.00671
    AIR           0.42807                       AIR          12.4852                     NOX            0.01057

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK          328.533            INDICATED POWER          9.582              NET WORK       0.200401
 INDICATED PUMP WORK     -54.375            INDICATED PUMP POWER    -1.586              HEAT LOSS      0.299590
 HEAT LOSS               409.854            HEAT LOSS RATE          11.954              EXHAUST        0.504170
 CHEM. ENERGY           1368.050            EXHAUST POWER           20.117

                                                    MISCELLANEOUS

                            INDICATED MEAN EFFECTIVE PRESSURE (ATM)               3.3560
                            PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -0.5554
                            MEAN TORQUE (NEWTON-METERS)                          21.8168

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1206.97 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.420
    AR        0.008638      CO        0.000487      CO2      0.115734      H2       0.000236      H2O       0.154329
    NO        0.000716      N2        0.719851      OH       0.000006

FRESH CHARGE MOLE FRACTIONS AT  279.78 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.514
    AR        0.000449      CO        0.000026      CO2      0.006009      H2       0.000012      H2O       0.008013
    NO        0.000038      N2        0.037377      C3H8     0.038123      AIR      0.909952

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=   8.621 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                                CYCLE   4    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1207.0 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                                   EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                                WT FRACTION    ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                      CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                   1.000000    -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                          1.000000       -29.792  G     298.15

                          A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

    TOTAL         0.47683                         CHARGE       12.9511                       EXHAUST       13.9790
    FUEL          0.02507                         FUEL          0.7377                       CO            0.00671
    AIR           0.39301                         AIR          11.5659                       NOX           0.01057
                                                  NET          12.8375                       NET           13.9790

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK          297.760             INDICATED POWER            8.685            NET WORK        0.169939
 INDICATED PUMP WORK     -84.225             INDICATED PUMP POWER      -2.457            HEAT LOSS       0.301741
 HEAT LOSS               379.147             HEAT LOSS RATE            11.058            EXHAUST         0.548914
 CHEM. ENERGY           1256.535             EXHAUST POWER             20.117
                                                       MISCELLANEOUS

                                    INDICATED MEAN EFFECTIVE PRESSURE (ATM)           3.0417
                                    PUMP MEAN EFFECTIVE PRESSURE (ATM)               -0.8604
                                    MEAN TORQUE (NEWTON-METERS)                      16.9925

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1206.97 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.420
    AR        0.008638      CO        0.000487      CO2       0.115734     H2        0.000236      H2O       0.154329
    NO        0.000716      N2        0.719851      OH        0.000006

FRESH CHARGE MOLE FRACTIONS AT  279.69 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.514
    AR        0.000449      CO        0.000025      CO2       0.006009     H2        0.000012      H2O       0.008013
    NO        0.000037      N2        0.037378      C3H8      0.038123     AIR       0.909953

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  56.562 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   5    LEVEL 5   CASE NO.       222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1240.0 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                         EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000
                                                                           WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                              1.000000   -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                    1.000000      -29.792  G     298.15

                  A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.45754                        CHARGE      11.8952                     EXHAUST      12.4854
     FUEL         0.02325                        FUEL         0.6775                     CO           0.01588
     AIR          0.36453                        AIR         10.6229                     NOX          0.00165
                                                 NET         11.9490                     NET          12.4853

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK          274.508           INDICATED POWER         8.006                NET WORK      0.164537
 INDICATED PUMP WORK     -82.183           INDICATED PUMP POWER   -2.397                HEAT LOSS     0.312701
 HEAT LOSS               365.514           HEAT LOSS RATE         10.661                EXHAUST       0.496479
 CHEM. ENERGY           1168.891           EXHAUST POWER          16.926

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                  2.8042
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                      -0.8395
                              MEAN TORQUE (NEWTON-METERS)                             15.3048

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1239.96 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.404
     AR       0.008633      CO       0.001290      CO2      0.114879      H        0.000013     H2        0.000484
     H2O      0.153975      NO       0.000125      N2       0.719748      OH       0.000056     O2        0.000794

FRESH CHARGE MOLE FRACTIONS AT  281.43 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.513
     AR       0.000448      CO       0.000067      CO2      0.005968      H2       0.000025     H2O       0.007999
     NO       0.000006      N2       0.037392      O2       0.000041      C3H8     0.038122     AIR       0.909926

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  66.835 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                       CYCLE   6    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1221.4 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000
                                                                              WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                   CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                                 1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                       1.000000      -29.792  G     298.15

                    A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                           PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

         TOTAL         0.45795                  CHARGE        11.9490                   EXHAUST       11.9486
         FUEL          0.02332                  FUEL           0.6806                   CO            0.01495
         AIR           0.36565                  AIR           10.6709                   NOX           0.00090
                                                NET           11.9463                   NET           11.9485

     ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK          275.399          INDICATED POWER          8.032              NET WORK       0.165012
 INDICATED PUMP WORK     -81.928          INDICATED PUMP POWER    -2.390              HEAT LOSS      0.312417
 HEAT LOSS               366.298          HEAT LOSS RATE          10.684              EXHAUST        0.465253
 CHEM. ENERGY           1172.466          EXHAUST POWER           15.910
                                                      MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.8133
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8369
                                   MEAN TORQUE (NEWTON-METERS)                        15.3959

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1221.43 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.405
     AR        0.008633      CO        0.001269      CO2       0.114861      H         0.000013     H2        0.000473
     H2O       0.153961      NO        0.000071      N2        0.719800      OH        0.000052     O2        0.000865

FRESH CHARGE MOLE FRACTIONS AT   280.45 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.513
     AR        0.000448      CO        0.000066      CO2       0.005967      H2        0.000025     H2O       0.007998
     N2        0.037393      O2        0.000045      C3H8      0.038122      AIR       0.909928

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  66.332 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE    7    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1224.6 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                               WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                    CAL/MOL            DEG K
FUEL    C  3.00000   H  8.00000                                                 1.000000   -24821.770  G      298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                       1.000000      -29.792  G      298.15

                     A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                       MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.45989                          CHARGE        12.0295                   EXHAUST       11.8587
     FUEL          0.02348                          FUEL           0.6852                   CO             0.01517
     AIR           0.36808                          AIR           10.7428                   NOX            0.00050
                                                    NET           12.0259                   NET           11.8586

   ENERGY PER CYCLE (JOULES)                  AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK          277.439             INDICATED POWER           8.092               NET WORK       0.165334
 INDICATED PUMP WORK     -82.344             INDICATED PUMP POWER     -2.402               HEAT LOSS      0.311512
 HEAT LOSS               367.584             HEAT LOSS RATE           10.721               EXHAUST        0.459960
 CHEM. ENERGY           1180.002             EXHAUST POWER            15.830

                                                        MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)                2.8341
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -0.8412
                               MEAN TORQUE (NEWTON-METERS)                           15.5251

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1224.58 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.404
     AR        0.008633      CO        0.001297      CO2       0.114873      H         0.000013      H2        0.000486
     H2O       0.153976      NO        0.000040      N2        0.719787      OH        0.000052      O2        0.000840

FRESH CHARGE MOLE FRACTIONS AT  280.62 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.513
     AR        0.000448      CO        0.000067      CO2       0.005968      H2        0.000025      H2O       0.007999
     N2        0.037394      O2        0.000044      C3H8      0.038122      AIR       0.909926

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  57.338 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                                    CYCLE   8    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1224.5 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                    EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000

                                                                                 WT FRACTION   ENERGY    STATE    TEMP
         CHEMICAL FORMULA                                                                      CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                                    1.000000   -24821.770  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                          1.000000      -29.792  G      298.15

                        A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.45828                        CHARGE        11.9366                      EXHAUST       11.9704
     FUEL          0.02332                        FUEL           0.6799                      CO            0.01517
     AIR           0.36565                        AIR           10.6599                      NOX           0.00044
                                                  NET           11.9362                      NET           11.9703

    ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK          275.522               INDICATED POWER           8.036              NET WORK      0.164935
 INDICATED PUMP WORK     -82.136               INDICATED PUMP POWER     -2.396              HEAT LOSS     0.312570
 HEAT LOSS               366.487               HEAT LOSS RATE           10.689              EXHAUST       0.467245
 CHEM. ENERGY           1172.497               EXHAUST POWER            15.979

                                                        MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)            2.8145
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                -0.8390
                                   MEAN TORQUE (NEWTON-METERS)                       15.3892

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1224.52 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.404
    AR        0.008633      CO          0.001285      CO2        0.114878      H          0.000013      H2         0.000482
    H2O       0.153978      NO          0.000035      N2         0.719797      OH         0.000052      O2         0.000844

FRESH CHARGE MOLE FRACTIONS AT  280.61 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.513
    AR        0.000448      CO          0.000067      CO2        0.005968      H2         0.000025      H2O        0.007999
    N2        0.037394      O2          0.000044      C3H8       0.038122      AIR        0.909927

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  61.720 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE   9    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1223.2 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000     B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.45719                         CHARGE      11.9370                     EXHAUST      11.9405
     FUEL          0.02325                         FUEL         0.6799                     CO           0.01504
     AIR           0.36452                         AIR         10.6603                     NOX          0.00041
                                                   NET         11.9432                     NET          11.9404

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK         274.612            INDICATED POWER           8.009              NET WORK       0.164576
 INDICATED PUMP WORK    -82.230            INDICATED PUMP POWER     -2.398              HEAT LOSS      0.312938
 HEAT LOSS              365.809            HEAT LOSS RATE           10.669              EXHAUST        0.466912
 CHEM. ENERGY          1168.953            EXHAUST POWER            15.919

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)            2.8052
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                -0.8400
                              MEAN TORQUE (NEWTON-METERS)                       15.3093

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1223.17 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.405
     AR        0.008633     CO        0.001277     CO2      0.114876     H        0.000013     H2       0.000477
     H2O       0.153974     NO        0.000032     N2       0.719807     OH       0.000052     O2       0.000856

FRESH CHARGE MOLE FRACTIONS AT  280.54 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.513
     AR        0.000448     CO        0.000066     CO2      0.005968     H2       0.000025     H2O      0.007999
     N2        0.037394     O2        0.000044     C3H8     0.038122     AIR      0.909927

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  63.188 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                     CYCLE  10    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.050     T(EGR) = 1222.7 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                               WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                    CAL/MOL          DEG K
FUEL     C  3.00000   H  8.00000                                                  1.000000   -24821.770  G    298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                        1.000000      -29.792  G    298.15

                         A/F= 15.6787   PERCENT FUEL=   5.9957   EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                           PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.45757                     CHARGE       11.8786                       EXHAUST      11.9567
     FUEL          0.02324                     FUEL          0.6766                       CO           0.01515
     AIR           0.36440                     AIR          10.6081                       NOX          0.00040
                                               NET          11.9067                       NET          11.9566

    ENERGY PER CYCLE (JOULES)             AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

  INDICATED WORK         274.379         INDICATED POWER          8.003              NET WORK       0.164465
  INDICATED PUMP WORK    -82.174         INDICATED PUMP POWER    -2.397              HEAT LOSS      0.312837
  HEAT LOSS              365.604         HEAT LOSS RATE          10.663              EXHAUST        0.467427
  CHEM. ENERGY          1168.670         EXHAUST POWER           15.933
                                                    MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8028
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8394
                                   MEAN TORQUE (NEWTON-METERS)                         15.2952

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1222.68 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.405
     AR        0.008633      CO        0.001285       CO2       0.114873      H         0.000013      H2         0.000482
     H2O       0.153972      NO        0.000031       N2        0.719801      OH        0.000052      O2         0.000855

FRESH CHARGE MOLE FRACTIONS AT  280.52 K  AND  0.4276 ATM       MOLECULAR WEIGHT =  29.513
     AR        0.000448      CO        0.000067       CO2       0.005968      H2        0.000025      H2O        0.007999
     N2        0.037394      O2        0.000044       C3H8      0.038122      AIR       0.909927

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  68.595 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  11    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050     T(EGR) = 1221.0 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                                 EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                              WT FRACTION   ENERGY   STATE   TEMP
        CHEMICAL FORMULA                                                                    CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                  1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                        1.000000      -29.792  G    298.15

                 A/F= 15.6787   PERCENT FUEL=   5.9957  EQUIVALENCE RATIO= 1.0000   PHI=   1.0000

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                    MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.45514                          CHARGE       11.7449                          EXHAUST       11.9551
     FUEL         0.02299                          FUEL          0.8022                          CO            0.01531
     AIR          0.36041                          AIR          10.4887                          NOX           0.00039
                                                   NET          11.8462                          NET           11.9551

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK         271.117              INDICATED POWER         7.908                  NET WORK      0.163698
 INDICATED PUMP WORK    -81.814              INDICATED PUMP POWER   -2.386                  HEAT LOSS     0.314226
 HEAT LOSS              363.376              HEAT LOSS RATE         10.598                  EXHAUST       0.471476
 CHEM. ENERGY          1156.417              EXHAUST POWER          15.902

                                                          MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.7695
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8357
                                   MEAN TORQUE (NEWTON-METERS)                        15.0642

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1221.04 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.404
     AR        0.008633       CO          0.001298      CO2       0.114872      H          0.000013       H2          0.000488
     H2O       0.153975       NO          0.000031      N2        0.719790      OH         0.000052       O2          0.000845

FRESH CHARGE MOLE FRACTIONS AT  280.70 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.622
     AR        0.000450       CO          0.000068      CO2       0.005990      H2         0.000025       H2O         0.008029
     N2        0.037533       O2          0.000044      C3H8      0.045343      AIR        0.902513

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  54.434 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  12    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1219.9 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                          EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000

                                                                           WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                            1.000000   -24821.770  G       298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  1.000000      -29.792  G       298.15

                         A/F= 13.0744   PERCENT FUEL=   7.1051   EQUIVALENCE RATIO= 1.1989   PHI=   1.1992

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46104                          CHARGE       12.0381                        EXHAUST      11.8010
     FUEL           0.02785                          FUEL          0.7890                        CO           0.01524
     AIR            0.36459                          AIR          10.6236                        NOX          0.00037
                                                     NET          12.0402                        NET          11.8010

    ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK          272.136             INDICATED POWER           7.937               NET WORK       0.158327
 INDICATED PUMP WORK     -82.856             INDICATED PUMP POWER     -2.417               HEAT LOSS      0.290437
 HEAT LOSS               347.217             HEAT LOSS RATE           10.127               EXHAUST        0.449657
 CHEM. ENERGY           1195.502             EXHAUST POWER            15.679
                                                           MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.7799
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8464
                              MEAN TORQUE (NEWTON-METERS)                         15.0624

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1219.87 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.404
     AR       0.008633      CO         0.001310      CO2      0.114864      H        0.000013      H2       0.000491
     H2O      0.153976      NO         0.000029      N2       0.719784      OH       0.000051      O2       0.000846

FRESH CHARGE MOLE FRACTIONS AT  280.59 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.603
     AR       0.000450      CO         0.000068      CO2      0.005986      H2       0.000026      H2O      0.008024
     N2       0.037509      O2         0.000044      C3H8     0.044093      AIR      0.903795

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  52.705 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE 13     LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1143.0 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000   A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG   FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G     298.15

                  A/F= 13.4641   PERCENT FUEL=   6.9137   EQUIVALENCE RATIO= 1.1642   PHI=   1.1645

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46053                         CHARGE       11.9525                       EXHAUST      12.0025
     FUEL         0.02690                         FUEL          0.7617                       CO           0.49072
     AIR          0.36209                         AIR          10.5698                       NOX          0.00022
                                                  NET          11.9515                       NET          12.0025

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK           272.096          INDICATED POWER          7.936              NET WORK      0.158703
 INDICATED PUMP WORK      -82.748          INDICATED PUMP POWER    -2.413              HEAT LOSS     0.291283
 HEAT LOSS                347.529          HEAT LOSS RATE          10.136              EXHAUST       0.492875
 CHEM. ENERGY            1193.101          EXHAUST POWER           17.151
                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)           2.7795
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)               -0.8453
                              MEAN TORQUE (NEWTON-METERS)                      15.0679

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1143.04 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  27.526
     AR        0.008283      CH4       0.000169      CO        0.040177      CO2       0.088012      C2H2      0.000850
     C2H4      0.000023      H2        0.016985      H2O       0.154874      NO        0.000016      N2        0.690598
     O2        0.000005

FRESH CHARGE MOLE FRACTIONS AT  277.06 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.535
     AR        0.000444      CH4       0.000009      CO        0.002155      CO2       0.004722      C2H2      0.000046
     H2        0.000911      H2O       0.008309      N2        0.037050      C3H8      0.042771      AIR       0.903579

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  56.435 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  14    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1144.7 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                         EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION    ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                  CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000    -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000       -29.792  G    298.15

                  A/F= 13.8768   PERCENT FUEL=   6.7219   EQUIVALENCE RATIO= 1.1297   PHI=   1.1299

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46263                      CHARGE      11.9770                       EXHAUST      11.9685
     FUEL         0.02625                      FUEL         0.8403                       CO           0.46450
     AIR          0.36420                      AIR         10.6133                       NOX          0.00021
                                               NET         12.0153                       NET          11.9685

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK        275.826             INDICATED POWER          8.045               NET WORK       0.160840
 INDICATED PUMP WORK   -83.024             INDICATED PUMP POWER    -2.422               HEAT LOSS      0.293576
 HEAT LOSS             351.915             HEAT LOSS RATE          10.264               EXHAUST        0.485561
 CHEM. ENERGY         1198.719             EXHAUST POWER           16.976
                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8176
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8481
                              MEAN TORQUE (NEWTON-METERS)                         15.3427

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1144.65 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.575
     AR       0.008302      CH4      0.000140      CO       0.038206      CO2      0.089404       C2H2     0.000739
     C2H4     0.000021      H2       0.015974      H2O      0.154944      NO       0.000016       N2       0.692240

FRESH CHARGE MOLE FRACTIONS AT  277.27 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.598
     AR       0.000446      CH4      0.000008      CO       0.002051      CO2      0.004798       C2H2     0.000040
     H2       0.000857      H2O      0.008316      N2       0.037152      C3H8     0.046784       AIR      0.899546

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  52.974 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                      CYCLE  15    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1156.9 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM      ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                                 EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000   A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000
                                                                          WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                              CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                             1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                   1.000000      -29.792  G     298.15

                  A/F= 12.6299   PERCENT FUEL=   7.3368   EQUIVALENCE RATIO= 1.2410   PHI=   1.2414

                                     PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.46436                      CHARGE       12.0451                     EXHAUST       12.1023
     FUEL          0.02879                      FUEL          0.7596                     CO            0.41042
     AIR           0.36394                      AIR          10.6033                     NOX           0.00023
                                                NET          12.0462                     NET           12.1022

    ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

  INDICATED WORK          270.403          INDICATED POWER           7.887           NET WORK       0.154543
  INDICATED PUMP WORK     -83.254          INDICATED PUMP POWER     -2.428           HEAT LOSS      0.280823
  HEAT LOSS               340.074          HEAT LOSS RATE            9.919           EXHAUST        0.481958
  CHEM. ENERGY           1210.988          EXHAUST POWER            17.023
                                                    MISCELLANEOUS

                             INDICATED MEAN EFFECTIVE PRESSURE (ATM)          2.7622
                             PUMP MEAN EFFECTIVE PRESSURE (ATM)              -0.8505
                             MEAN TORQUE (NEWTON-METERS)                     14.8929

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1156.86 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.682
     AR        0.008346     CH4       0.000083     CO        0.033515     CO2       0.092745     C2H2      0.000552
     C2H4      0.000014     H2        0.013689     H2O       0.155159     NO        0.000017     N2        0.695867

FRESH CHARGE MOLE FRACTIONS AT  277.68 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.540
     AR        0.000445     CO        0.001788     CO2       0.004949     C2H2      0.000029     H2        0.000730
     H2O       0.008279     N2        0.037129     C3H8      0.042545     AIR       0.904098

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  50.365 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  16    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.050      T(EGR) = 1117.9 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                            EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =       0.000000   C2 = 0.387200E 00   C3 =       0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000    0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL     C  3.00000   H  8.00000                                               1.000000   -24821.770  G    298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                     1.000000      -29.792  G    298.15

                  A/F= 13.9587   PERCENT FUEL=   6.6851   EQUIVALENCE RATIO= 1.1230   PHI=   1.1232

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46387                         CHARGE       12.0391                         EXHAUST      12.0997
     FUEL         0.02623                         FUEL          0.7179                         CO           0.63231
     AIR          0.36577                         AIR          10.6725                         NOX          0.00015
                                                  NET          12.0367                         NET          12.0996

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK         277.371            INDICATED POWER        8.090                  NET WORK       0.161128
 INDICATED PUMP WORK    -83.065            INDICATED PUMP POWER  -2.423                  HEAT LOSS      0.292381
 HEAT LOSS              352.585            HEAT LOSS RATE        10.284                  EXHAUST        0.504199
 CHEM. ENERGY          1205.910            EXHAUST POWER         17.734

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8334
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8485
                              MEAN TORQUE (NEWTON-METERS)                         15.4624

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1117.89 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.256
     AR        0.008174     CH4        0.000321      CO         0.050850      CO2        0.080615      C2H2       0.001406
     C2H4      0.000041     H2         0.022940      H2O        0.154131      NO         0.000011      N2         0.681496
     O2        0.000007

FRESH CHARGE MOLE FRACTIONS AT  275.82 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.478
     AR        0.000442     CH4        0.000017      CO         0.002750      CO2        0.004359      C2H2       0.000076
     H2        0.001241     H2O        0.008335      N2         0.036854      C3H8       0.040026      AIR        0.905895

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  55.056 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  17    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1159.6 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                         EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F= 14.8664   PERCENT FUEL=   6.3026   EQUIVALENCE RATIO= 1.0546   PHI=   1.0546

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46358                      CHARGE       12.0359                      EXHAUST      12.0862
     FUEL         0.02472                      FUEL          0.6412                      CO           0.41255
     AIR          0.36727                      AIR          10.7135                      NOX          0.00023
                                               NET          12.0360                      NET          12.0862

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK        281.101             INDICATED POWER         8.199                NET WORK      0.165711
 INDICATED PUMP WORK   -82.530             INDICATED PUMP POWER   -2.407                HEAT LOSS     0.301866
 HEAT LOSS             361.725             HEAT LOSS RATE         10.550                EXHAUST       0.487902
 CHEM. ENERGY         1198.295             EXHAUST POWER          17.052

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.8715
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8431
                              MEAN TORQUE (NEWTON-METERS)                        15.8018

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1159.60 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  27.682
     AR       0.008346      CH4      0.000087      CO       0.033734      CO2      0.092545      C2H2     0.000547
     C2H4     0.000014      H2       0.013769      H2O      0.155085      NO       0.000017      N2       0.695843

FRESH CHARGE MOLE FRACTIONS AT  277.54 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.439
     AR       0.000444      CO       0.001794      CO2      0.004921      C2H2     0.000029      H2       0.000732
     H2O      0.008246      N2       0.037000      C3H8     0.035814      AIR      0.911013

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  50.674 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                       CYCLE  18    LEVEL 5    CASE NO.       222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1189.0 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =   966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                              EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =       0.000000   C2 = 0.387200E 00   C3 =       0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG     FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                               WT FRACTION    ENERGY    STATE    TEMP
         CHEMICAL FORMULA                                                                    CAL/MOL             DEG K
FUEL     C  3.00000   H  8.00000                                                 1.000000   -24821.770  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                       1.000000      -29.792  G      298.15

                    A/F= 16.7088    PERCENT FUEL=    5.6469    EQUIVALENCE RATIO= 0.9384    PHI=    0.9383

                                           PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                       MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46133                        CHARGE       12.0152                        EXHAUST       12.0928
     FUEL           0.02213                        FUEL          0.5606                        CO            0.23049
     AIR            0.36933                        AIR          10.7699                        NOX           0.00032
                                                   NET          12.0135                        NET           12.0928

   ENERGY PER CYCLE (JOULES)                    AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK          271.271             INDICATED POWER            7.912               NET WORK       0.166023
 INDICATED PUMP WORK     -82.686             INDICATED PUMP POWER      -2.412               HEAT LOSS      0.314328
 HEAT LOSS               357.043             HEAT LOSS RATE            10.414               EXHAUST        0.499017
 CHEM. ENERGY           1135.894             EXHAUST POWER             16.533

                                                       MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)                 2.7711
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                     -0.8447
                               MEAN TORQUE (NEWTON-METERS)                            15.0071

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1188.96 K   AND   1.0000 ATM      MOLECULAR WEIGHT =  28.018
     AR          0.008479       CH4        0.000007       CO         0.019065       CO2        0.102870       C2H2        0.000143
     H           0.000005       H2         0.007368       H2O        0.155058       NO         0.000025       N2          0.706967
     O2          0.000007

FRESH CHARGE MOLE FRACTIONS AT  278.70 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.389
     AR          0.000445       CO         0.001000       CO2        0.005395       C2H2       0.000007       H2          0.000386
     H2O         0.008132       N2         0.037079       C3H8       0.031324       AIR        0.916227

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  51.006 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                  CYCLE  19    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1198.6 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                              EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                             1.000000   -24821.770  G      298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                   1.000000      -29.792  G      298.15

                           A/F= 19.2130   PERCENT FUEL=   4.9473   EQUIVALENCE RATIO= 0.8163   PHI=   0.8160

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL         0.45835                         CHARGE        11.9535                        EXHAUST       12.0307
     FUEL          0.01922                         FUEL           0.5848                        CO            0.00179
     AIR           0.36883                         AIR           10.7940                        NOX           0.00034
                                                   NET           11.9596                        NET           12.0306

   ENERGY PER CYCLE (JOULES)                   AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK           237.116            INDICATED POWER           6.916               NET WORK       0.158064
 INDICATED PUMP WORK      -83.743            INDICATED PUMP POWER     -2.443               HEAT LOSS      0.323661
 HEAT LOSS                314.054            HEAT LOSS RATE            9.160               EXHAUST        0.540916
 CHEM. ENERGY             970.320            EXHAUST POWER            15.308

                                                          MISCELLANEOUS

                                     INDICATED MEAN EFFECTIVE PRESSURE (ATM)                 2.4222
                                     PUMP MEAN EFFECTIVE PRESSURE (ATM)                     -0.8555
                                     MEAN TORQUE (NEWTON-METERS)                            12.2051

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1198.57 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.446
     AR        0.008666       CO         0.000151      CO2       0.112015      H2        0.000026      H2O       0.149117
     NO        0.000026       N2         0.722504      OH        0.000060      O2        0.007430

FRESH CHARGE MOLE FRACTIONS AT  278.85 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.431
     AR        0.000448       CO         0.000008      CO2       0.005795      H2O       0.007714      N2        0.037376
     O2        0.000384       C3H8       0.032589      AIR       0.915679

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  55.930 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                     CYCLE  20    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1101.7 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                                EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                                 WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                      CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                     1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                           1.000000      -29.792  G    298.15

                           A/F= 18.4566   PERCENT FUEL=   5.1396   EQUIVALENCE RATIO= 0.8497   PHI=   0.8495

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                           MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL           0.46126                            CHARGE        11.9047                     EXHAUST       11.8376
     FUEL            0.01986                            FUEL           0.6554                     CO            0.00070
     AIR             0.36672                            AIR           10.7282                     NOX           0.00012
                                                        NET           11.9027                     NET           11.8376

   ENERGY PER CYCLE (JOULES)                        AVERAGE ENERGY RATE - POWER (KW)                   CYCLE EFFICIENCIES

 INDICATED WORK           243.343                 INDICATED POWER           7.098                NET WORK        0.160549
 INDICATED PUMP WORK      -83.419                 INDICATED PUMP POWER     -2.433                HEAT LOSS       0.320848
 HEAT LOSS                319.601                 HEAT LOSS RATE            9.322                EXHAUST         0.450635
 CHEM. ENERGY             996.112                 EXHAUST POWER            13.092
                                                              MISCELLANEOUS

                                       INDICATED MEAN EFFECTIVE PRESSURE (ATM)            2.4858
                                       PUMP MEAN EFFECTIVE PRESSURE (ATM)                -0.8521
                                       MEAN TORQUE (NEWTON-METERS)                       12.7264

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1101.66 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.507
    AR        0.008746       CO          0.000060       CO2         0.099332      H2O       0.132098      NO          0.000009
    N2        0.729222       OH          0.000033       O2          0.030495

FRESH CHARGE MOLE FRACTIONS AT  273.49 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.495
    AR        0.000452       CO2         0.005139       H2O         0.006834      N2        0.037725      O2          0.001578
    C3H8      0.036586       AIR         0.911680

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  50.804 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE  21    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1115.2 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM       STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                   EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS    C1 =       0.000000   C2 = 0.387200E 00    C3 =       0.000000     A =  0.4000     B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG     FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.375000  -0.500000    0.125000

                                                                                   WT FRACTION    ENERGY    STATE    TEMP
        CHEMICAL FORMULA                                                                          CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                                      1.000000    -24821.770  G      298.15
AIR      N  1.56168   O  0.41959    AR 0.00936    C  0.00032                          1.000000       -29.792  G      298.15

                          A/F= 16.3682    PERCENT FUEL=    5.7577   EQUIVALENCE RATIO= 0.9579    PHI=    0.9579

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                          MEAN INLET MASS FLOW RATE (G/SEC)          MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL           0.46795                               CHARGE        12.0899                          EXHAUST        12.0130
     FUEL            0.02264                               FUEL           0.7258                          CO              0.00062
     AIR             0.37097                               AIR           10.8241                          NOX             0.00011
                                                           NET           12.0913                          NET            12.0129

   ENERGY PER CYCLE (JOULES)                      AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK            274.096            INDICATED POWER             7.994                NET WORK        0.168441
 INDICATED PUMP WORK       -82.835            INDICATED PUMP POWER       -2.416                HEAT LOSS       0.311879
 HEAT LOSS                 354.132            HEAT LOSS RATE             10.329                EXHAUST         0.408609
 CHEM. ENERGY             1135.479            EXHAUST POWER              13.532
                                                          MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)                  2.8000
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                      -0.8462
                                   MEAN TORQUE (NEWTON-METERS)                             15.2201

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1115.22 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.502
     AR         0.008739      CO          0.000052      CO2         0.100379      H2O       0.133490       NO          0.000009
     N2         0.728681      OH          0.000035      O2          0.028609

FRESH CHARGE MOLE FRACTIONS AT  274.37 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.546
     AR         0.000453      CO2         0.005203      H2O         0.006919      N2        0.037769       O2          0.001483
     C3H8       0.039998      AIR         0.908170

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  60.836 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  22    LEVEL 5    CASE NO.       222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1186.7 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000    0.125000

                                                                               WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                     CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                  1.000000    -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                        1.000000       -29.792  G     298.15

                              A/F= 14.9144   PERCENT FUEL=   6.2836   EQUIVALENCE RATIO= 1.0512   PHI=   1.0512

                                               PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                      MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46641                         CHARGE        12.1319                         EXHAUST       12.1925
     FUEL           0.02481                         FUEL           0.6580                         CO             0.00108
     AIR            0.37022                         AIR           10.8011                         NOX            0.00030
                                                    NET           12.1300                         NET           12.1925

   ENERGY PER CYCLE (JOULES)                   AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK          286.322              INDICATED POWER            8.351              NET WORK      0.168482
 INDICATED PUMP WORK     -82.755              INDICATED PUMP POWER      -2.414              HEAT LOSS     0.306656
 HEAT LOSS               370.515              HEAT LOSS RATE            10.807              EXHAUST       0.432059
 CHEM. ENERGY           1208.244              EXHAUST POWER             15.226
                                                              MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.9248
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8454
                              MEAN TORQUE (NEWTON-METERS)                         16.1994

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1186.75 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.458
     AR         0.008681       CO         0.000090       CO2        0.109723       H2         0.000013       H2O        0.145985
     NO         0.000023       N2         0.723764       OH         0.000058       O2         0.011660

FRESH CHARGE MOLE FRACTIONS AT  278.29 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.491
     AR         0.000450       CO2        0.005685       H2O        0.007564       N2         0.037501       O2         0.000604
     C3H8       0.036484       AIR        0.911700

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  46.534 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  23    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1219.4 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                         EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000   A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC   BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F= 16.4142   PERCENT FUEL=   5.7425   EQUIVALENCE RATIO= 0.9553   PHI=   0.9552

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46114                      CHARGE       12.0185                     EXHAUST      12.2254
     FUEL         0.02250                      FUEL          0.6327                     CO           0.09939
     AIR          0.36909                      AIR          10.7619                     NOX          0.00041
                                               NET          12.0148                     NET          12.2253

   ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK        271.347            INDICATED POWER         7.914                NET WORK      0.156869
 INDICATED PUMP WORK   -82.745            INDICATED PUMP POWER   -2.413                HEAT LOSS     0.297322
 HEAT LOSS             357.467            HEAT LOSS RATE         10.426                EXHAUST       0.471391
 CHEM. ENERGY         1202.291            EXHAUST POWER          16.530
                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.7719
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8453
                              MEAN TORQUE (NEWTON-METERS)                        15.0085

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1219.36 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.253
     AR       0.008572      CO       0.008200      CO2      0.110518      H        0.000010      H2       0.003213
     H2O      0.154686      NO       0.000032      N2       0.714708      OH       0.000006      O2       0.000051

FRESH CHARGE MOLE FRACTIONS AT  280.33 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.461
     AR       0.000447      CO       0.000428      CO2      0.005762      H2       0.000168      H2O      0.008065
     N2       0.037263      C3H8     0.035243      AIR      0.912618

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  50.815 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                       CYCLE  24    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1200.1 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS    C1 =      0.000000   C2 = 0.387200E 00    C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG     FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                              WT FRACTION    ENERGY   STATE    TEMP
             CHEMICAL FORMULA                                                                CAL/MOL            DEG K
FUEL     C  3.00000   H  8.00000                                                1.000000    -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000       -29.792  G     298.15

                          A/F= 17.0094    PERCENT FUEL=    5.5527    EQUIVALENCE RATIO= 0.9219    PHI=    0.9218

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

           MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

          TOTAL          0.45798                          CHARGE       11.8787                       EXHAUST       12.0322
          FUEL           0.02150                          FUEL          0.7460                       CO            0.00185
          AIR            0.36551                          AIR          10.6581                       NOX           0.00035
                                                          NET          11.8899                       NET           12.0321

         ENERGY PER CYCLE (JOULES)                  AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK          260.406                 INDICATED POWER          7.595                  NET WORK        0.164384
 INDICATED PUMP WORK     -82.579                 INDICATED PUMP POWER    -2.409                  HEAT LOSS       0.318749
 HEAT LOSS               344.817                 HEAT LOSS RATE          10.057                  EXHAUST         0.486147
 CHEM. ENERGY           1081.780                 EXHAUST POWER           15.339

                                                           MISCELLANEOUS

                                    INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.6601
                                    PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8436
                                    MEAN TORQUE (NEWTON-METERS)                         14.1510

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1200.10 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.446
     AR          0.008665       CO          0.000156       CO2        0.112104       H2         0.000027       H2O       0.149234
     NO          0.000027       N2          0.722455       OH         0.000061       O2         0.007267

FRESH CHARGE MOLE FRACTIONS AT   279.29 K  AND   0.4276 ATM      MOLECULAR WEIGHT =   29.569
     AR          0.000450       CO          0.000008       CO2        0.005826       H2O        0.007756       N2        0.037549
     O2          0.000378       C3H8        0.041672       AIR        0.906354

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  57.030 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                   CYCLE  25    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1173.5 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                 EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS    C1 =      0.000000    C2 = 0.387200E 00    C3 =      0.000000    A =  0.4000     B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.375000  -0.500000    0.125000

                                                                                WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                      CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                                  1.000000    -24821.770  G      298.15
AIR      N  1.56168   O  0.41959    AR 0.00936    C  0.00032                      1.000000       -29.792  G      298.15

                           A/F= 14.2866    PERCENT FUEL=   6.5417   EQUIVALENCE RATIO= 1.0973    PHI=   1.0974

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                        MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46167                           CHARGE        11.9575                          EXHAUST        11.8947
     FUEL           0.02547                           FUEL           0.6628                          CO             0.00097
     AIR            0.36433                           AIR           10.6166                          NOX            0.00027
                                                      NET           11.9568                          NET            11.8946

   ENERGY PER CYCLE (JOULES)                     AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK          279.154                INDICATED POWER          8.142                 NET WORK       0.153619
 INDICATED PUMP WORK     -82.674                INDICATED PUMP POWER    -2.411                 HEAT LOSS      0.282290
 HEAT LOSS               361.050                HEAT LOSS RATE          10.531                 EXHAUST        0.391681
 CHEM. ENERGY           1279.003                EXHAUST POWER           14.611

                                                           MISCELLANEOUS

                                      INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8516
                                      PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8445
                                      MEAN TORQUE (NEWTON-METERS)                         15.6353

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1173.55 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.463
     AR        0.008687        CO          0.000083        CO2        0.108788        H2         0.000011       H2O        0.144730
     NO        0.000021        N2          0.724262        OH         0.000052        O2         0.013364

FRESH CHARGE MOLE FRACTIONS AT  277.59 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.504
     AR        0.000450        CO2         0.005638        H2O        0.007501        N2         0.037538       O2         0.000693
     C3H8      0.037349        AIR         0.910820

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  50.407 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                     CYCLE  26    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1191.4 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =   966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                             WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                  CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                 1.000000   -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                       1.000000      -29.792  G     298.15

                          A/F= 16.0186   PERCENT FUEL=   5.8759   EQUIVALENCE RATIO= 0.9788   PHI=   0.9788

                                             PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46125                          CHARGE       11.9773                          EXHAUST       12.1145
     FUEL         0.02297                          FUEL          0.8271                          CO             0.23076
     AIR          0.36760                          AIR          10.7098                          NOX            0.00033
                                                   NET          12.0147                          NET           12.1145

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK          276.580             INDICATED POWER          8.067                   NET WORK      0.166344
 INDICATED PUMP WORK     -82.361             INDICATED PUMP POWER    -2.402                   HEAT LOSS     0.312491
 HEAT LOSS               364.856             HEAT LOSS RATE          10.642                   EXHAUST       0.487498
 CHEM. ENERGY           1167.575             EXHAUST POWER           16.601
                                                       MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8253
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8413
                                   MEAN TORQUE (NEWTON-METERS)                         15.4555

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1191.37 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.018
     AR         0.008479     CH4        0.000007      CO         0.019053      CO2        0.102871      C2H2       0.000149
     H          0.000005     H2         0.007357      H2O        0.155066      NO         0.000025      N2         0.706973
     O2         0.000008

FRESH CHARGE MOLE FRACTIONS AT  279.39 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.607
     AR         0.000448     CO         0.001007      CO2        0.005435      C2H2       0.000008      H2         0.000389
     H2O        0.008193     N2         0.037353      C3H8       0.045728      AIR        0.901436

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  53.131 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                       CYCLE  27    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050     T(EGR) = 1217.0 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                                EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000     B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                             WT FRACTION   ENERGY   STATE   TEMP
        CHEMICAL FORMULA                                                                   CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G     298.15

                     A/F= 12.9487   PERCENT FUEL=   7.1691   EQUIVALENCE RATIO= 1.2105   PHI=   1.2108

                                          PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

    TOTAL        0.46195                       CHARGE        12.0489                        EXHAUST       12.0468
    FUEL         0.02811                       FUEL           0.7832                        CO             0.00545
    AIR          0.36452                       AIR           10.6258                        NOX            0.00039
                                               NET           12.0500                        NET           12.0466

   ENERGY PER CYCLE (JOULES)               AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

 INDICATED WORK        271.908          INDICATED POWER          7.931               NET WORK       0.157378
 INDICATED PUMP WORK   -83.136          INDICATED PUMP POWER    -2.425               HEAT LOSS      0.288148
 HEAT LOSS             345.628          HEAT LOSS RATE          10.081               EXHAUST        0.450848
 CHEM. ENERGY         1199.483          EXHAUST POWER           15.773

                                                       MISCELLANEOUS

                                   INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.7776
                                   PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8492
                                   MEAN TORQUE (NEWTON-METERS)                        15.0220

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1216.97 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.428
     AR        0.008647       CO         0.000459      CO2      0.114422       H2       0.000120       H2O       0.152629
     NO        0.000030       N2         0.720935      OH       0.000062       O2       0.002690

FRESH CHARGE MOLE FRACTIONS AT  280.37 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.599
     AR        0.000450       CO         0.000024      CO2      0.005957       H2       0.000006       H2O       0.007946
     N2        0.037532       O2         0.000140      C3H8     0.043776       AIR      0.904162

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  49.435 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE  28     LEVEL 5    CASE NO.       222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5       RPM = 3500.0      EGR = 0.050      T(EGR) = 1136.5 K      SPARK ADVANCE =   20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =   966.13 CC      CHAMBER AREA =129.030 SQ CM      WALL TEMP =   360.0 K

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                               EVOPEN = 465.00 DEG      EVSHUT =   45.00 DEG

HEAT TRANSFER PARAMETERS    C1 =      0.000000    C2 = 0.387200E 00    C3 =      0.000000     A =  0.4000     B =  0.8000

    KINETIC FLAME     FINITE BURNING INTERVAL =109.5 DEG     FOURIER COMBUSTION     TAU =     0.0000 SEC     BETA =    0.000
         AN =     0.375000   -0.500000    0.125000

                                                                              WT FRACTION    ENERGY    STATE    TEMP
         CHEMICAL FORMULA                                                                    CAL/MOL            DEG K
FUEL     C  3.00000    H  8.00000                                               1.000000    -24821.770   G      298.15
AIR      N  1.56168    O  0.41959    AR 0.00936 . C  0.00032                    1.000000       -29.792   G      298.15

                    A/F= 13.5669    PERCENT FUEL=    6.8649    EQUIVALENCE RATIO= 1.1554    PHI=    1.1557

                                            PERFORMANCE PARAMETERS FOR ONE CYLINDER

       MASS PER CYCLE (G)                      MEAN INLET MASS FLOW RATE (G/SEC)          MEAN EXHAUST MASS FLOW RATE (G/SEC)

       TOTAL           0.46155                       CHARGE          11.9838                      EXHAUST        12.0551
       FUEL            0.02681                       FUEL             0.6552                      CO              0.52096
       AIR             0.36360                       AIR             10.6031                      NOX             0.00020
                                                     NET             11.9812                      NET            12.0550

     ENERGY PER CYCLE (JOULES)                  AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK            274.051             INDICATED POWER              7.993            NET WORK        0.159672
 INDICATED PUMP WORK       -82.812             INDICATED PUMP POWER        -2.415            HEAT LOSS       0.291808
 HEAT LOSS                 349.497             HEAT LOSS RATE              10.194            EXHAUST         0.494980
 CHEM. ENERGY             1197.697             EXHAUST POWER               17.291

                                                        MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                     2.7995
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                         -0.8459
                              MEAN TORQUE (NEWTON-METERS)                                15.2183

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1136.55 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.472
     AR         0.008261       CH4        0.000198       CO         0.042384      CO2        0.086472      C2H2       0.000955
     C2H4       0.000024       H2         0.018142       H2O        0.154764      NO         0.000015      N2         0.688771
     O2         0.000005

FRESH CHARGE MOLE FRACTIONS AT  276.52 K  AND  0.4276 ATM      MOLECULAR WEIGHT =   29.444
     AR         0.000443       CH4        0.000011       CO         0.002271      CO2        0.004634      C2H2       0.000051
     H2         0.000972       H2O        0.008294       N2         0.036910      C3H8       0.036914      AIR        0.909497
NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  48.432 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                          CYCLE  29    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1151.4 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP-=  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                               EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =   0.375000  -0.500000   0.125000

                                                                                WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                     CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                                  1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959   AR 0.00936   C  0.00032                        1.000000      -29.792  G     298.15

                   A/F= 16.1841   PERCENT FUEL=   5.8193   EQUIVALENCE RATIO= 0.9688   PHI=   0.9688

                                           PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

    TOTAL         0.46325                          CHARGE       12.0413                         EXHAUST      11.9734
    FUEL          0.02290                          FUEL          0.6754                         CO            0.44791
    AIR           0.37004                          AIR          10.7735                         NOX           0.00022
                                                   NET          12.0586                         NET          11.9733

   ENERGY PER CYCLE (JOULES)               AVERAGE ENERGY RATE - POWER (KW)              CYCLE EFFICIENCIES

 INDICATED WORK         280.950           INDICATED POWER          8.194            NET WORK      0.166254
 INDICATED PUMP WORK    -82.566           INDICATED PUMP POWER    -2.408            HEAT LOSS     0.309200
 HEAT LOSS              368.957           HEAT LOSS RATE          10.761            EXHAUST       0.488225
 CHEM. ENERGY          1193.264           EXHAUST POWER           16.992

                                                   MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                2.8700
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -0.8434
                              MEAN TORQUE (NEWTON-METERS)                           15.7870

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1151.41 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.607
     AR         0.008316       CH4        0.000124       CO        0.036870       CO2        0.090338       C2H2        0.000683
     C2H4       0.000018       H2         0.015297       H2O       0.154999       NO         0.000017       N2          0.693329

FRESH CHARGE MOLE FRACTIONS AT  277.23 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.459
     AR         0.000444       CH4        0.000007       CO        0.001967       CO2        0.004820       C2H2        0.000036
     H2         0.000816       H2O        0.008270       N2        0.036992       C3H8       0.037439       AIR         0.909206

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  52.658 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                      CYCLE  30    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5       RPM = 3500.0      EGR = 0.050     T(EGR) = 1228.6 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                          EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                       WT FRACTION   ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                            CAL/MOL           DEG K
FUEL     C  3.00000   H  8.00000                                         1.000000   -24821.770  G     298.15
AIR      N  1.56168   O  0.41959    AR 0.00936    C  0.00032             1.000000      -29.792  G     298.15

                         A/F= 15.9518    PERCENT FUEL=    5.8991    EQUIVALENCE RATIO= 0.9829    PHI=    0.9829

                                           PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46078                        CHARGE         12.0118                      EXHAUST       12.1154
     FUEL           0.02307                        FUEL            0.7171                      CO            0.01342
     AIR            0.36797                        AIR            10.7380                      NOX           0.00040
                                                   NET            12.0123                      NET           12.1153

   ENERGY PER CYCLE (JOULES)                 AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

  INDICATED WORK          276.784            INDICATED POWER          8.073                  NET WORK      0.165970
  INDICATED PUMP WORK     -82.381            INDICATED PUMP POWER    -2.403                  HEAT LOSS     0.312348
  HEAT LOSS               365.857            HEAT LOSS RATE          10.671                  EXHAUST       0.474391
  CHEM. ENERGY           1171.311            EXHAUST POWER           16.207

                                                      MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                2.8274
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -0.8415
                              MEAN TORQUE (NEWTON-METERS)                           15.4701

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1228.58 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.409
     AR         0.008635      CO         0.001124      CO2        0.114906      H          0.000011     H2           0.000404
     H2O        0.153877      NO         0.000031      N2         0.719963      OH         0.000054     O2           0.000992

FRESH CHARGE MOLE FRACTIONS AT  280.89 K  AND  0.4276 ATM       MOLECULAR WEIGHT =  29.539
     AR         0.000449      CO         0.000058      CO2        0.005974      H2         0.000021     H2O          0.008000
     N2         0.037430      O2         0.000052      C3H8       0.039837      AIR        0.908173

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  56.716 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  31    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1219.4 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                           EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F= 14.9745   PERCENT FUEL=   6.2600   EQUIVALENCE RATIO= 1.0470   PHI=   1.0470

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46033                          CHARGE     12.0201                        EXHAUST      12.0477
     FUEL         0.02451                          FUEL        0.7491                        CO           0.00760
     AIR          0.36724                          AIR        10.7043                        NOX          0.00039
                                                   NET        12.0159                        NET          12.0476

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK         279.340            INDICATED POWER         8.147                    NET WORK      0.166259
 INDICATED PUMP WORK    -82.458            INDICATED PUMP POWER   -2.405                    HEAT LOSS     0.308626
 HEAT LOSS              365.473            HEAT LOSS RATE         10.660                    EXHAUST       0.459233
 CHEM. ENERGY          1184.192            EXHAUST POWER          15.861

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                 2.8535
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                     -0.8423
                              MEAN TORQUE (NEWTON-METERS)                            15.6674

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1219.38 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.422
     AR        0.008643      CO        0.000640      CO2      0.114725      H2       0.000188      H2O       0.153207
     NO        0.000031      N2        0.720585      OH       0.000059      O2       0.001915

FRESH CHARGE MOLE FRACTIONS AT  280.44 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.567
     AR        0.000450      CO        0.000033      CO2      0.005967      H2       0.000010      H2O       0.007969
     N2        0.037481      O2        0.000100      C3H8     0.041663      AIR      0.906322

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  53.251 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                   CYCLE  32    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1205.1 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                             EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
         AN =    0.375000  -0.500000   0.125000

                                                                       WT FRACTION    ENERGY    STATE    TEMP
         CHEMICAL FORMULA                                                             CAL/MOL            DEG K
FUEL    C  3.00000   H  8.00000                                          1.000000    -24821.770   G      298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                1.000000       -29.792   G      298.15

                   A/F= 14.2893   PERCENT FUEL=   6.5405   EQUIVALENCE RATIO= 1.0971   PHI=   1.0972

                                              PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                    MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.45992                       CHARGE        11.9752                      EXHAUST       12.0288
     FUEL           0.02551                       FUEL           0.6873                      CO            0.12769
     AIR            0.36468                       AIR           10.6323                      NOX           0.00039
                                                  NET           11.9760                      NET           12.0287

    ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                  CYCLE EFFICIENCIES

 INDICATED WORK        276.329              INDICATED POWER          8.060                 NET WORK      0.163531
 INDICATED PUMP WORK   -82.648              INDICATED PUMP POWER    -2.411                 HEAT LOSS     0.302202
 HEAT LOSS             357.920              HEAT LOSS RATE          10.439                 EXHAUST       0.468467
 CHEM. ENERGY         1184.374              EXHAUST POWER           16.183

                                                        MISCELLANEOUS

                             INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8228
                             PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8443
                             MEAN TORQUE (NEWTON-METERS)                         15.4127

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1205.14 K  AND  1.0000 ATM       MOLECULAR WEIGHT =  28.200
     AR        0.008551      CO        0.010687      CO2       0.108777      C2H2      0.000018      H         0.000008
     H2        0.004134      H2O       0.154787      NO        0.000030      N2        0.712969      O2        0.000032

FRESH CHARGE MOLE FRACTIONS AT  279.74 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.509
     AR        0.000447      CO        0.000559      CO2       0.005691      H2        0.000216      H2O       0.008099
     N2        0.037303      C3H8      0.038601      AIR       0.909077

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  49.227 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  33    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1181.6 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                         EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000

                                                                            WT FRACTION   ENERGY   STATE   TEMP
         CHEMICAL FORMULA                                                                 CAL/MOL          DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000   -24821.770  G    298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000      -29.792  G    298.15

                  A/F= 15.4694   PERCENT FUEL=   6.0719   EQUIVALENCE RATIO= 1.0135   PHI=   1.0135

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                   MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL        0.46022                          CHARGE       11.9768                     EXHAUST      12.0401
     FUEL         0.02370                          FUEL          0.8403                     CO           0.27106
     AIR          0.36640                          AIR          10.6871                     NOX          0.00031
                                                   NET          11.9751                     NET          12.0401

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                CYCLE EFFICIENCIES

 INDICATED WORK          278.905             INDICATED POWER           8.135               NET WORK      0.165989
 INDICATED PUMP WORK     -82.700             INDICATED PUMP POWER     -2.412               HEAT LOSS     0.310107
 HEAT LOSS               366.559             HEAT LOSS RATE           10.691               EXHAUST       0.480548
 CHEM. ENERGY           1182.040             EXHAUST POWER            16.567

                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)                  2.8491
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                      -0.8448
                              MEAN TORQUE (NEWTON-METERS)                             15.6135

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1181.61 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.942
     AR        0.008449      CH4      0.000018      CO        0.022458      CO2       0.100465      C2H2      0.000231
     C2H4      0.000006      H        0.000005      H2        0.008766      H2O       0.155121      NO        0.000024
     N2        0.704448      O2       0.000006

FRESH CHARGE MOLE FRACTIONS AT  278.96 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.615
     AR        0.000448      CO       0.001190      CO2       0.005324      C2H2      0.000012      H2        0.000465
     H2O       0.008220      N2       0.037331      C3H8      0.046506      AIR       0.900499

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  46.828 SEC
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INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  34     LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0      EGR = 0.050     T(EGR) = 1213.6 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                            EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000

                                                                            WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                  CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                1.000000    -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                      1.000000       -29.792  G     298.15

                  A/F= 12.7189   PERCENT FUEL=   7.2892   EQUIVALENCE RATIO= 1.2324   PHI=   1.2327

                                      PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46106                     CHARGE       11.9843                      EXHAUST        12.0359
     FUEL           0.02841                     FUEL          0.6593                      CO             0.07685
     AIR            0.36191                     AIR          10.5552                      NOX            0.00039
                                                NET          11.9888                      NET            12.0359

   ENERGY PER CYCLE (JOULES)                AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK         268.763             INDICATED POWER         7.839                NET WORK       0.155563
 INDICATED PUMP WORK    -82.967             INDICATED PUMP POWER   -2.420                HEAT LOSS      0.285845
 HEAT LOSS              341.397             HEAT LOSS RATE          9.957                EXHAUST        0.461720
 CHEM. ENERGY          1194.345             EXHAUST POWER          16.084
                                                    MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)               2.7455
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                   -0.8475
                              MEAN TORQUE (NEWTON-METERS)                          14.7852

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1213.58 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  28.290
     AR        0.008587      CO        0.006448      CO2       0.111731      H         0.000014      H2        0.002589
     H2O       0.154587      NO        0.000031      N2        0.715916      OH        0.000009      O2        0.000087

FRESH CHARGE MOLE FRACTIONS AT  280.09 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.495
     AR        0.000448      CO        0.000336      CO2       0.005825      H2        0.000135      H2O       0.008059
     N2        0.037321      C3H8      0.037359      AIR       0.910510

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  47.021 SEC
```
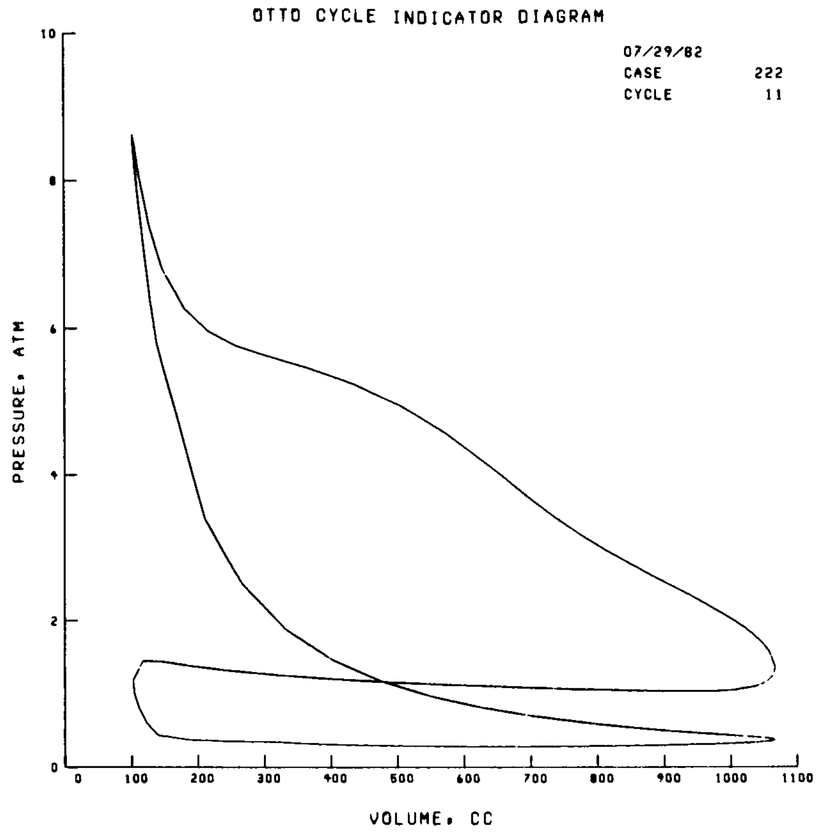
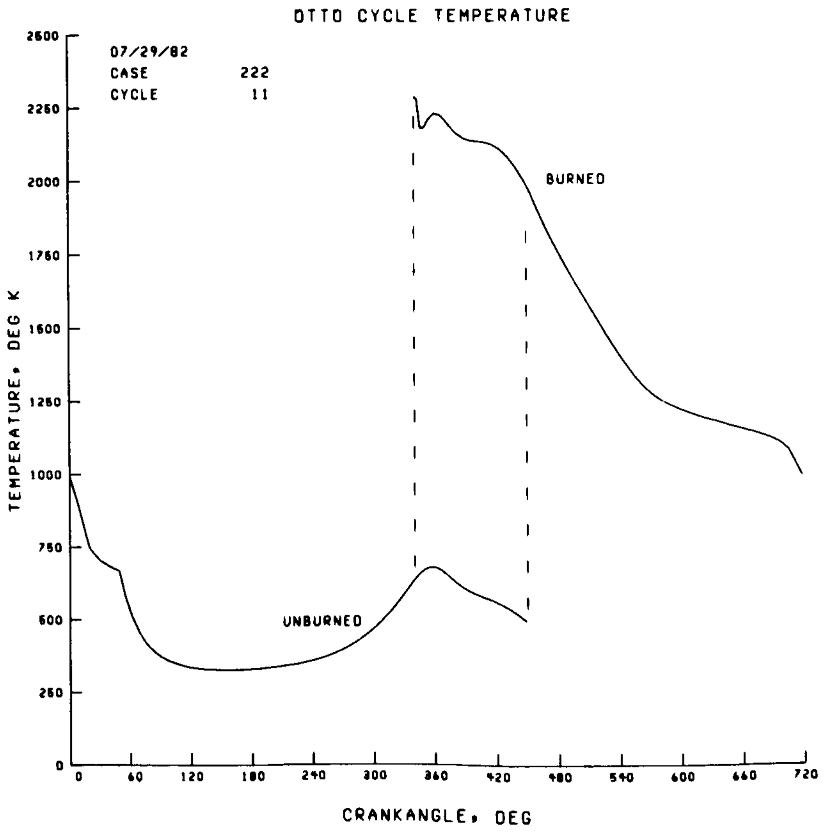

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                    CYCLE  35    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1124.8 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                               EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000    A =  0.4000     B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =     0.0000 SEC    BETA =   0.000
         AN =   0.375000  -0.500000   0.125000

                                                                              WT FRACTION    ENERGY   STATE    TEMP
         CHEMICAL FORMULA                                                                    CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                 1.000000    -24821.770  G     298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                       1.000000       -29.792  G     298.15

                  A/F= 16.0090   PERCENT FUEL=   5.8793   EQUIVALENCE RATIO= 0.9794   PHI=   0.9794

                                         PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                     MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.45543                        CHARGE        11.8930                       EXHAUST        11.9773
     FUEL           0.02258                        FUEL           0.7430                       CO             0.57045
     AIR            0.36075                        AIR           10.6341                       NOX            0.00018
                                                   NET           11.9131                       NET           11.9773

   ENERGY PER CYCLE (JOULES)                  AVERAGE ENERGY RATE - POWER (KW)                 CYCLE EFFICIENCIES

 INDICATED WORK           274.632              INDICATED POWER          8.010                 NET WORK        0.164867
 INDICATED PUMP WORK      -82.255              INDICATED PUMP POWER    -2.399                 HEAT LOSS       0.312401
 HEAT LOSS                364.528              HEAT LOSS RATE          10.632                 EXHAUST         0.508911
 CHEM. ENERGY            1166.860              EXHAUST POWER           17.320

                                                       MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)             2.8054
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                 -0.8403
                              MEAN TORQUE (NEWTON-METERS)                        15.3089

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1124.84 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.367
    AR          0.008218        CH4         0.000259        CO          0.046533        CO2         0.083584        C2H2          0.001180
    C2H4        0.000032        H2          0.020441        H2O         0.154489        NO          0.000014        N2            0.685234
    O2          0.000007

FRESH CHARGE MOLE FRACTIONS AT  276.17 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.507
    AR          0.000443        CH4         0.000014        CO          0.002509        CO2         0.004506        C2H2          0.000064
    H2          0.001102        H2O         0.008329        N2          0.036941        C3H8        0.041513        AIR           0.904576

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  58.337 SEC
```

```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                CYCLE  36    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5     RPM = 3500.0     EGR = 0.050     T(EGR) = 1223.7 K     SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM     MANIFOLD PRESSURE = 0.42760 ATM     EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM     STROKE = 10.312 CM     ROD = 17.145 CM     CHAMBER AREA =129.030 SQ CM     WALL TEMP_=  360.0 K
TOTAL VOLUME = 1067.83 CC     DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG     IVSHUT = 265.00 DEG                                EVOPEN = 465.00 DEG     EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =     0.000000   C2 = 0.387200E 00   C3 =     0.000000    A =  0.4000    B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =    0.000
        AN =   0.375000  -0.500000   0.125000

                                                                          WT FRACTION   ENERGY   STATE    TEMP
        CHEMICAL FORMULA                                                                CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                            1.000000   -24821.770  G       298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                  1.000000      -29.792  G       298.15

                    A/F= 14.3130   PERCENT FUEL=   6.5304   EQUIVALENCE RATIO= 1.0953   PHI=   1.0954

                                       PERFORMANCE PARAMETERS FOR ONE CYLINDER

      MASS PER CYCLE (G)                  MEAN INLET MASS FLOW RATE (G/SEC)        MEAN EXHAUST MASS FLOW RATE (G/SEC)

     TOTAL          0.46256                     CHARGE        12.0416                     EXHAUST       11.9257
     FUEL           0.02561                     FUEL           0.6656                     CO            0.03128
     AIR            0.36686                     AIR           10.6924                     NOX           0.00038
                                                NET           12.0332                     NET           11.9256

    ENERGY PER CYCLE (JOULES)              AVERAGE ENERGY RATE - POWER (KW)                   CYCLE EFFICIENCIES

  INDICATED WORK         278.439        INDICATED POWER          8.121                NET WORK      0.163977
  INDICATED PUMP WORK    -82.674        INDICATED PUMP POWER    -2.411                HEAT LOSS     0.299905
  HEAT LOSS              358.043        HEAT LOSS RATE          10.443                EXHAUST       0.453612
  CHEM. ENERGY          1193.856        EXHAUST POWER           15.795

                                                     MISCELLANEOUS

                               INDICATED MEAN EFFECTIVE PRESSURE (ATM)                2.8443
                               PUMP MEAN EFFECTIVE PRESSURE (ATM)                    -0.8445
                               MEAN TORQUE (NEWTON-METERS)                           15.5785

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1223.66 K  AND  1.0000 ATM     MOLECULAR WEIGHT =  28.371
     AR        0.008619      CO        0.002657      CO2      0.114251      H         0.000025      H2          0.001139
     H2O       0.154308      NO        0.000030      N2       0.718619      OH        0.000034      O2          0.000316

FRESH CHARGE MOLE FRACTIONS AT  280.57 K  AND  0.4276 ATM     MOLECULAR WEIGHT =  29.498
     AR        0.000448      CO        0.000138      CO2      0.005939      H2        0.000059      H2O         0.008022
     N2        0.037357      O2        0.000016      C3H8     0.037243      AIR       0.910771

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  51.482 SEC
```

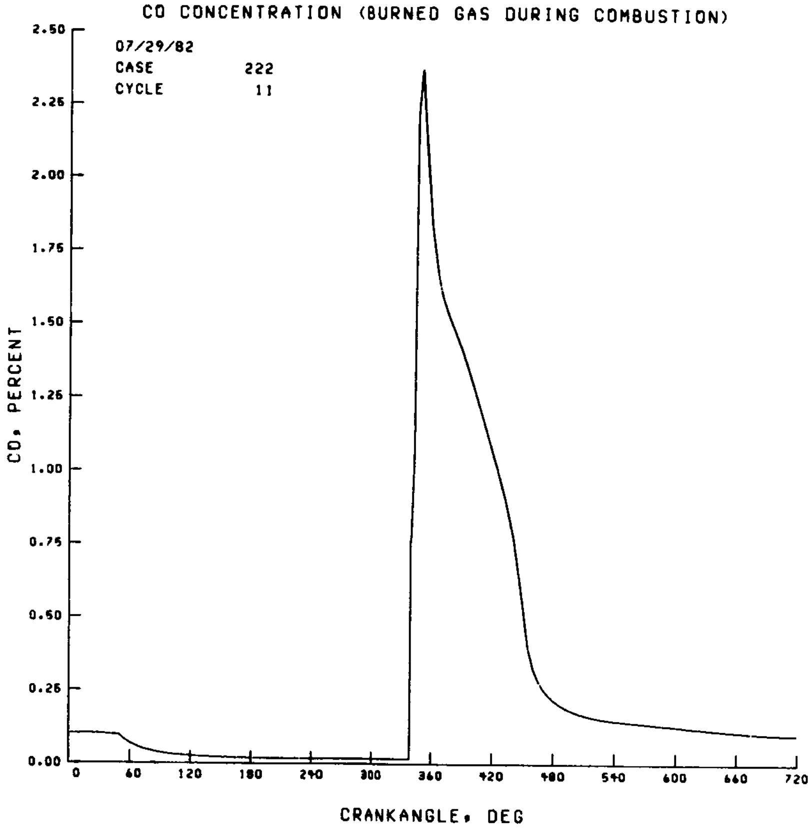
```
INTERNAL COMBUSTION ENGINE MODEL ZMOTTO                                            CYCLE  37    LEVEL 5    CASE NO.      222
    REF:  ZELEZNIK, FRANK J.; AND MCBRIDE, BONNIE J.:  MODELING THE INTERNAL COMBUSTION ENGINE. NASA RP-1094, 1985.

COMPRESSION RATIO =  10.5      RPM = 3500.0      EGR = 0.050      T(EGR) = 1175.4 K      SPARK ADVANCE =  20.00 DEG
FUEL PRESSURE = 1.00000 ATM      MANIFOLD PRESSURE = 0.42760 ATM      EXHAUST PRESSURE = 1.00000 ATM
FLOWS ARE ISENTROPIC
BORE = 10.922 CM      STROKE = 10.312 CM      ROD = 17.145 CM      CHAMBER AREA =129.030 SQ CM      WALL TEMP =  360.0 K
TOTAL VOLUME = 1067.83 CC      DISPLACEMENT VOLUME =  966.13 CC

IVOPEN = 699.00 DEG      IVSHUT = 265.00 DEG                              EVOPEN = 465.00 DEG      EVSHUT =  45.00 DEG

HEAT TRANSFER PARAMETERS   C1 =      0.000000   C2 = 0.387200E 00   C3 =      0.000000     A =  0.4000     B =  0.8000

    KINETIC FLAME    FINITE BURNING INTERVAL =109.5 DEG    FOURIER COMBUSTION    TAU =    0.0000 SEC    BETA =   0.000
         AN =    0.375000  -0.500000   0.125000

                                                                                 WT FRACTION   ENERGY   STATE    TEMP
        CHEMICAL FORMULA                                                                       CAL/MOL           DEG K
FUEL    C  3.00000   H  8.00000                                                    1.000000   -24821.770  G      298.15
AIR     N  1.56168   O  0.41959   AR 0.00936   C  0.00032                          1.000000      -29.792  G      298.15

                A/F= 16.0636   PERCENT FUEL=   5.8604  EQUIVALENCE RATIO= 0.9761   PHI=   0.9760

                                       PERFORMANCE PARAMETERS FOR ONE CYLINDER

     MASS PER CYCLE (G)                 MEAN INLET MASS FLOW RATE (G/SEC)       MEAN EXHAUST MASS FLOW RATE (G/SEC)

    TOTAL          0.45916                   CHARGE       11.9479                      EXHAUST       12.0619
    FUEL           0.02280                   FUEL          0.5391                      CO            0.28410
    AIR            0.36585                   AIR          10.6853                      NOX           0.00030
                                             NET          11.9463                      NET           12.0618

   ENERGY PER CYCLE (JOULES)            AVERAGE ENERGY RATE - POWER (KW)               CYCLE EFFICIENCIES

  INDICATED WORK          274.746       INDICATED POWER           8.013            NET WORK       0.165404
  INDICATED PUMP WORK     -82.279       INDICATED PUMP POWER     -2.400            HEAT LOSS      0.313104
  HEAT LOSS               364.335       HEAT LOSS RATE           10.626            EXHAUST        0.488056
  CHEM. ENERGY           1163.623       EXHAUST POWER            16.564

                                                   MISCELLANEOUS

                              INDICATED MEAN EFFECTIVE PRESSURE (ATM)              2.8066
                              PUMP MEAN EFFECTIVE PRESSURE (ATM)                  -0.8405
                              MEAN TORQUE (NEWTON-METERS)                         15.3161

COMPOSITE EXHAUST GAS MOLE FRACTIONS AT 1175.38 K  AND  1.0000 ATM      MOLECULAR WEIGHT =  27.919
     AR        0.008440      CH4        0.000021      CO         0.023476      CO2        0.099745      C2H2       0.000255
     C2H4      0.000006      H2         0.009181      H2O        0.155141      NO         0.000023      N2         0.703697
     O2        0.000005

FRESH CHARGE MOLE FRACTIONS AT  278.01 K  AND  0.4276 ATM      MOLECULAR WEIGHT =  29.370
     AR        0.000444      CO         0.001235      CO2        0.005246      C2H2       0.000013      H2         0.000483
     H2O       0.008160      N2         0.037013      C3H8       0.030390      AIR        0.917011

NOTE:  INLET AND EXHAUST VALUES CALCULATED WHEN THE VALVES CLOSE.

COMPUTER CYCLE TIME=  65.169 SEC
```

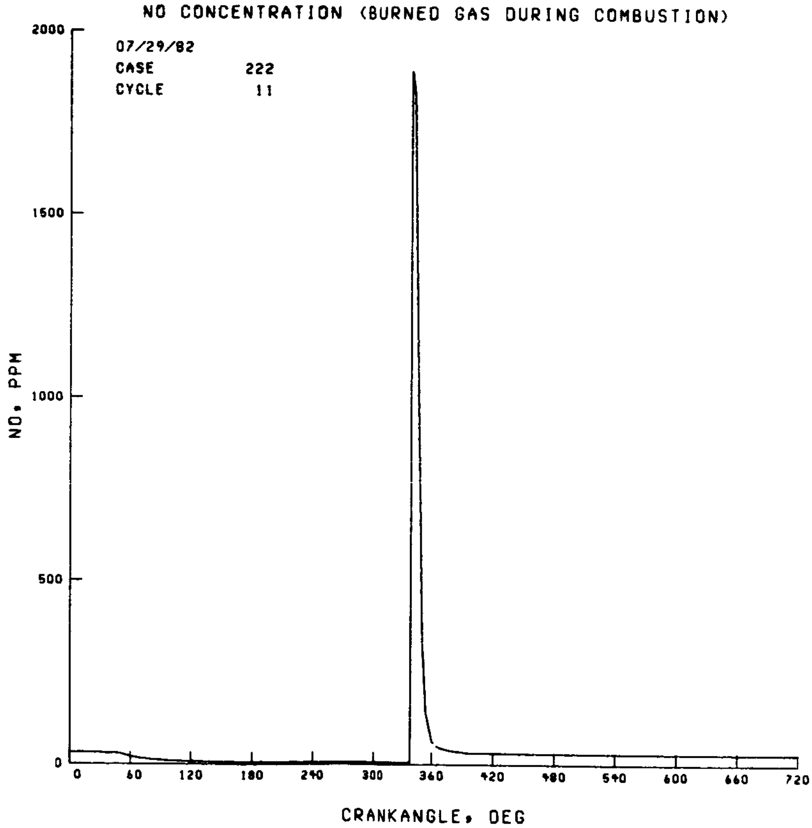


OTTO CYCLE INDICATOR DIAGRAM

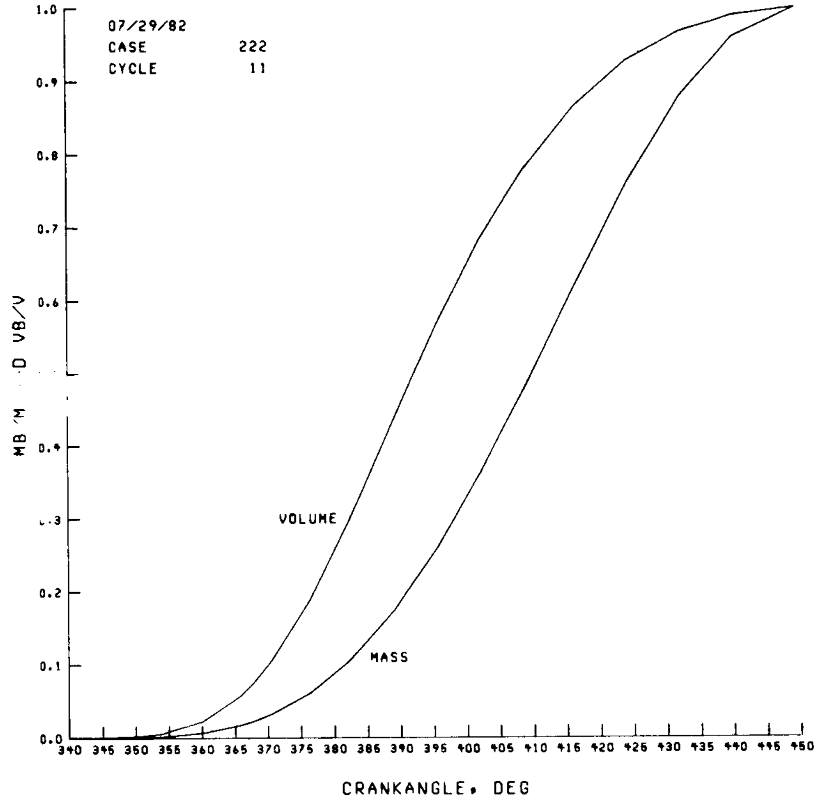


OTTO CYCLE TEMPERATURE

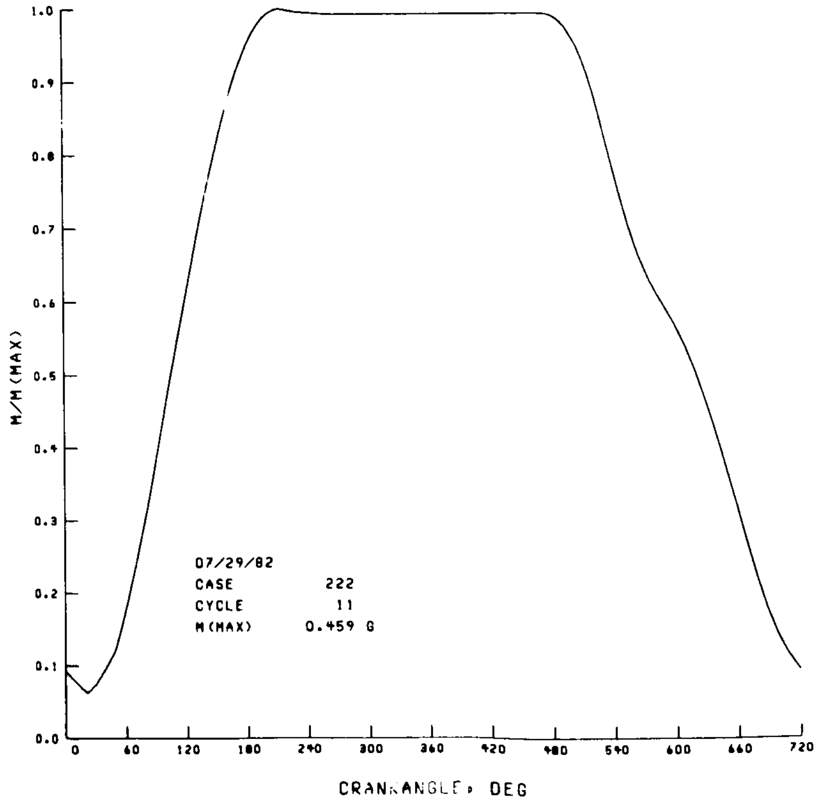

CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 11
CO, PERCENT
2.50
2.25
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

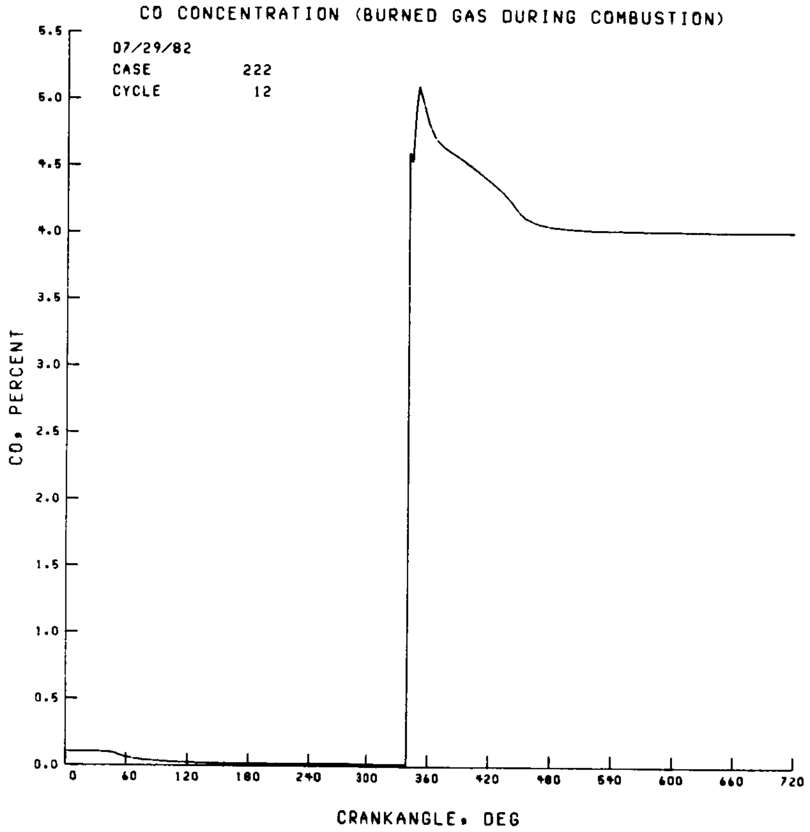

NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 11
NO, PPM
2000
1500
1000
500
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

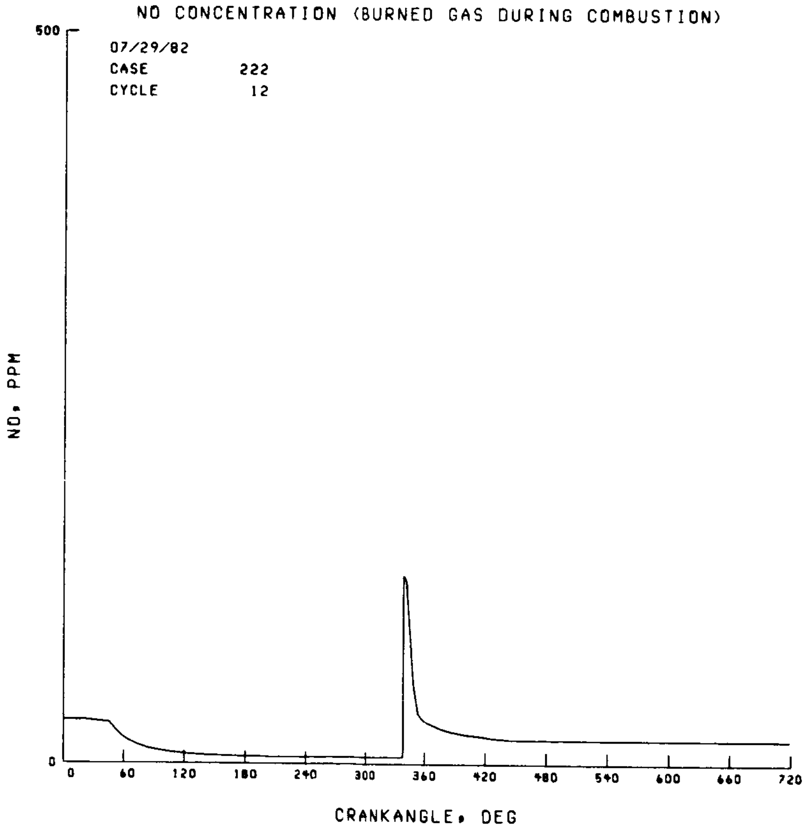
OTTO CYCLE BURNED MASS AND VOLUME FRACTIONS

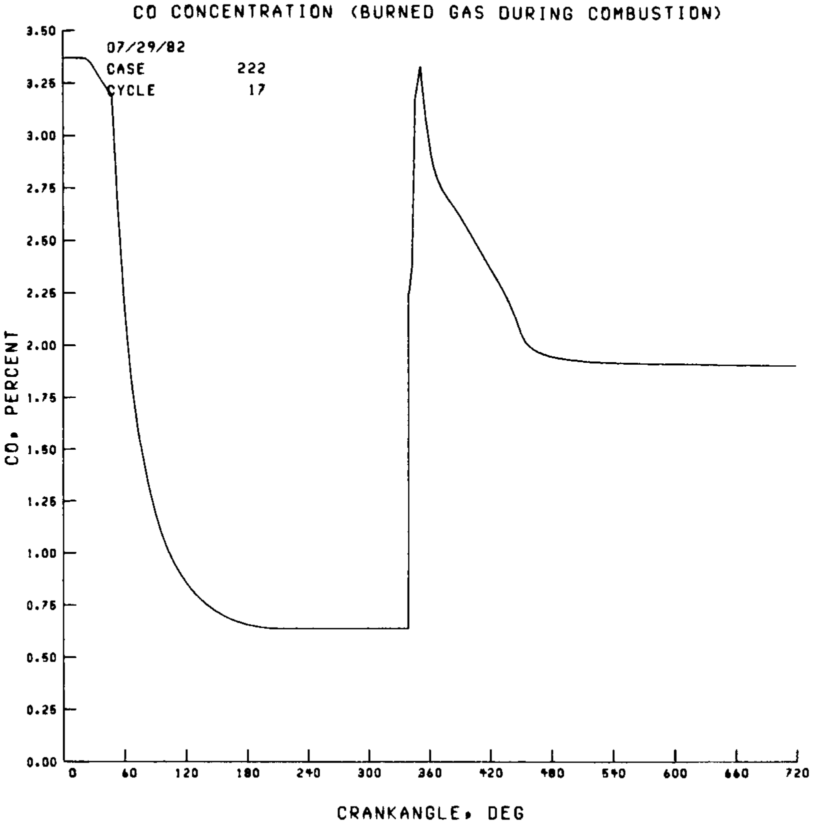


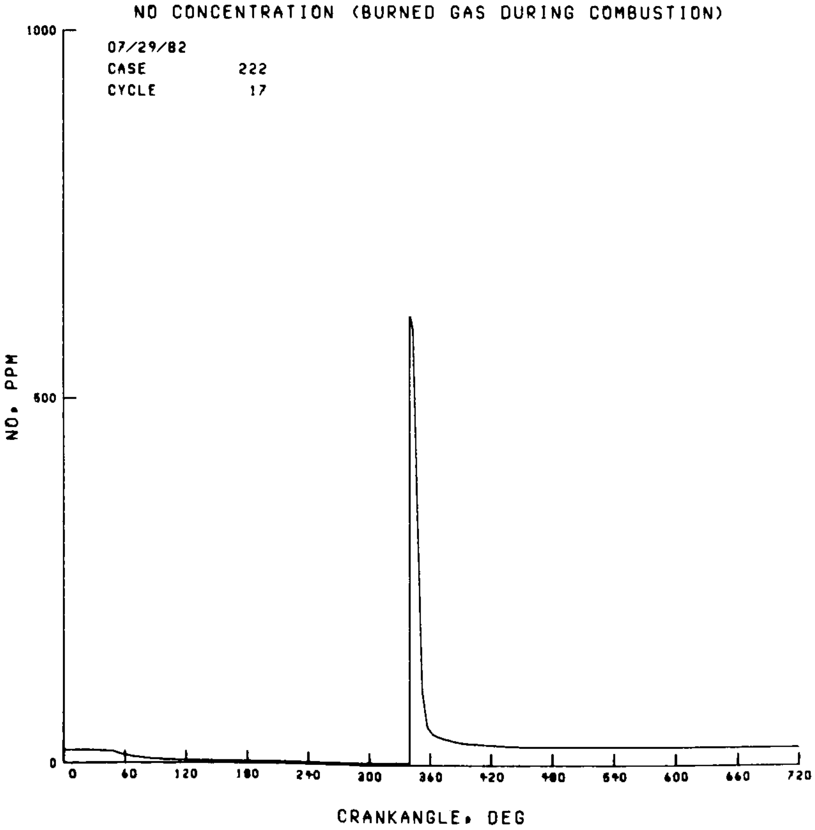
OTTO CYCLE MASS



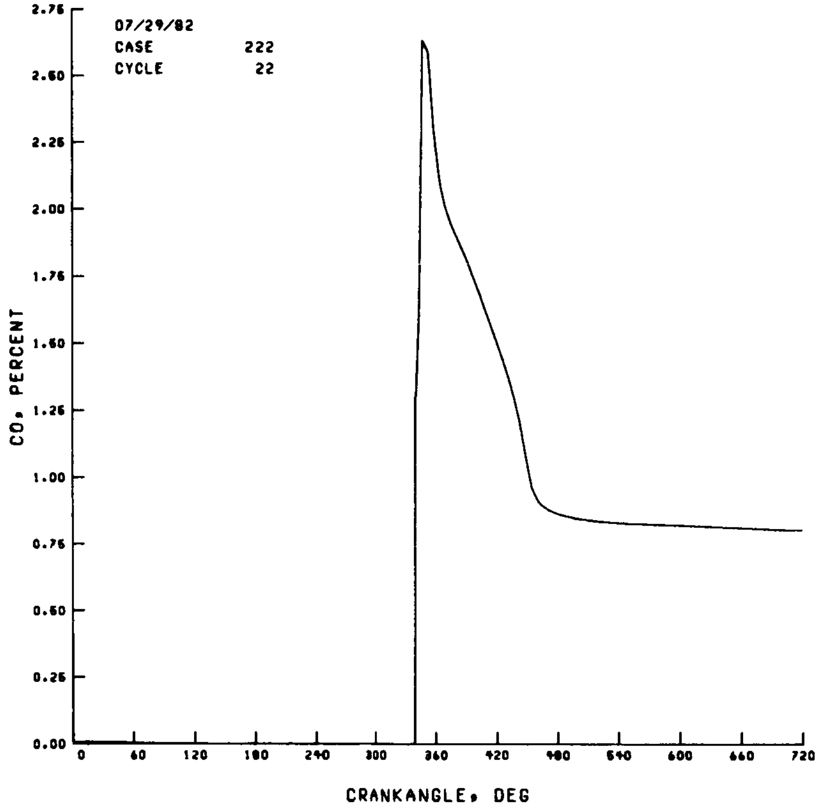

CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 12
CO, PERCENT
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 12
NO, PPM
500
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

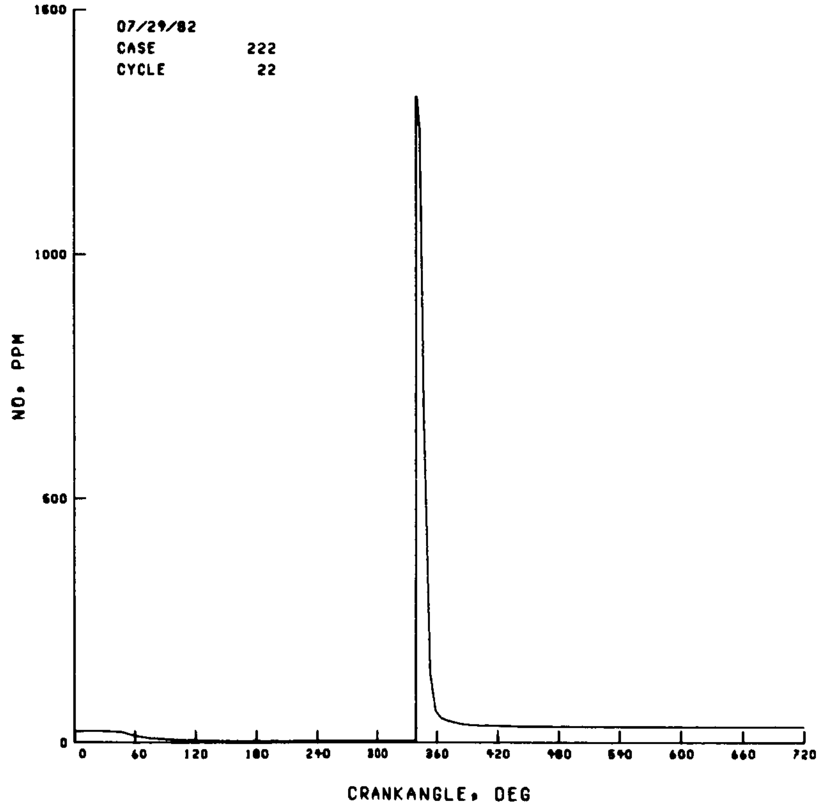

CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 17
CO, PERCENT
3.50
3.25
3.00
2.75
2.50
2.25
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

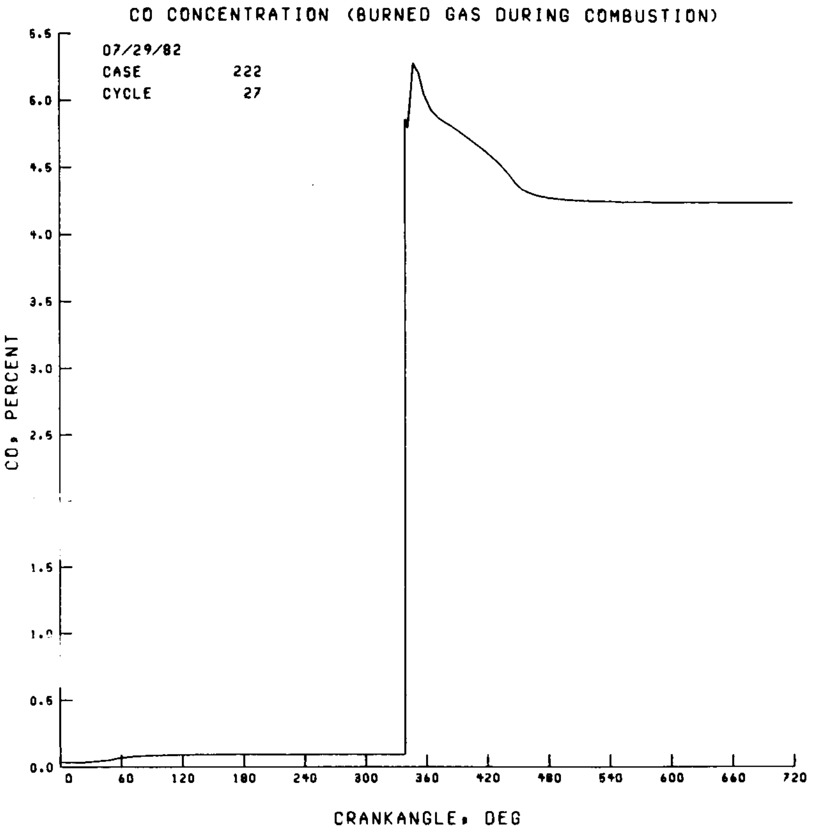

NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 17
NO, PPM
1000
500
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

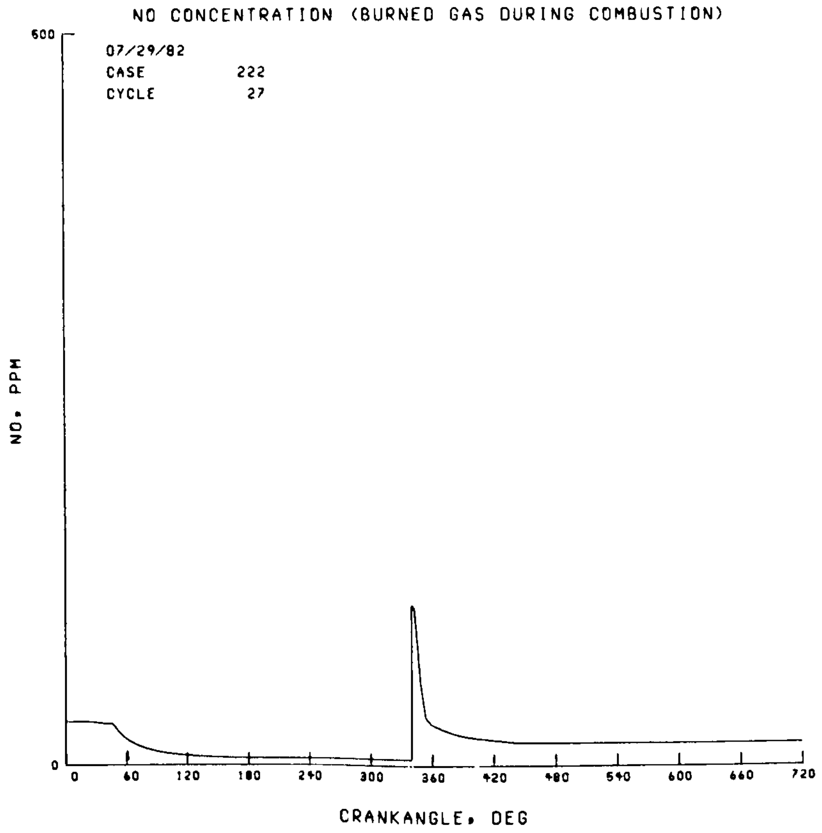
CO CONCENTRATION (BURNED GAS DURING COMBUSTION)

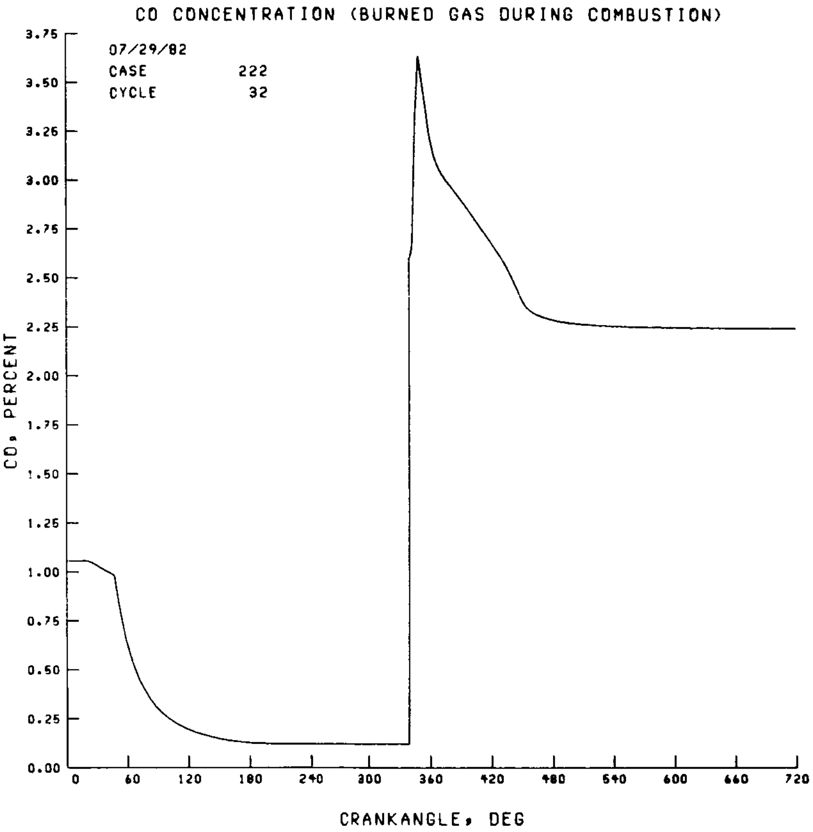


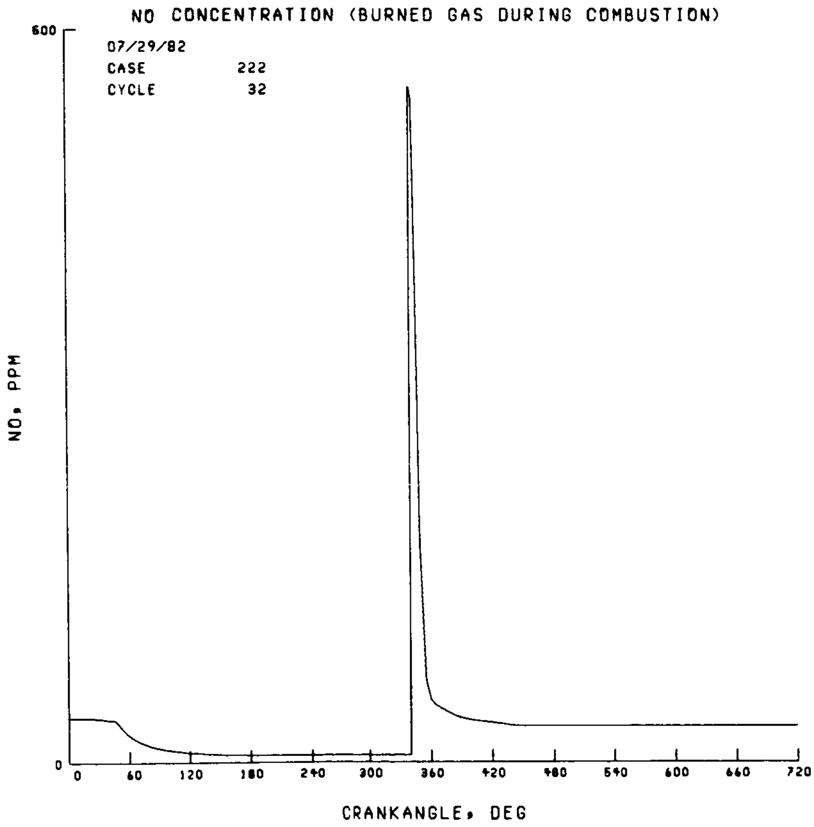
NO CONCENTRATION (BURNED GAS DURING COMBUSTION)




CO CONCENTRATION (BURNED GAS DURING COMBUSTION)


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)


CO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 32
CO, PERCENT
3.75
3.50
3.25
3.00
2.75
2.50
2.25
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG


NO CONCENTRATION (BURNED GAS DURING COMBUSTION)
07/29/82
CASE 222
CYCLE 32
NO, PPM
600
0
0
60
120
180
240
300
360
420
480
540
600
660
720
CRANKANGLE, DEG

Appendix J

Flow Diagrams

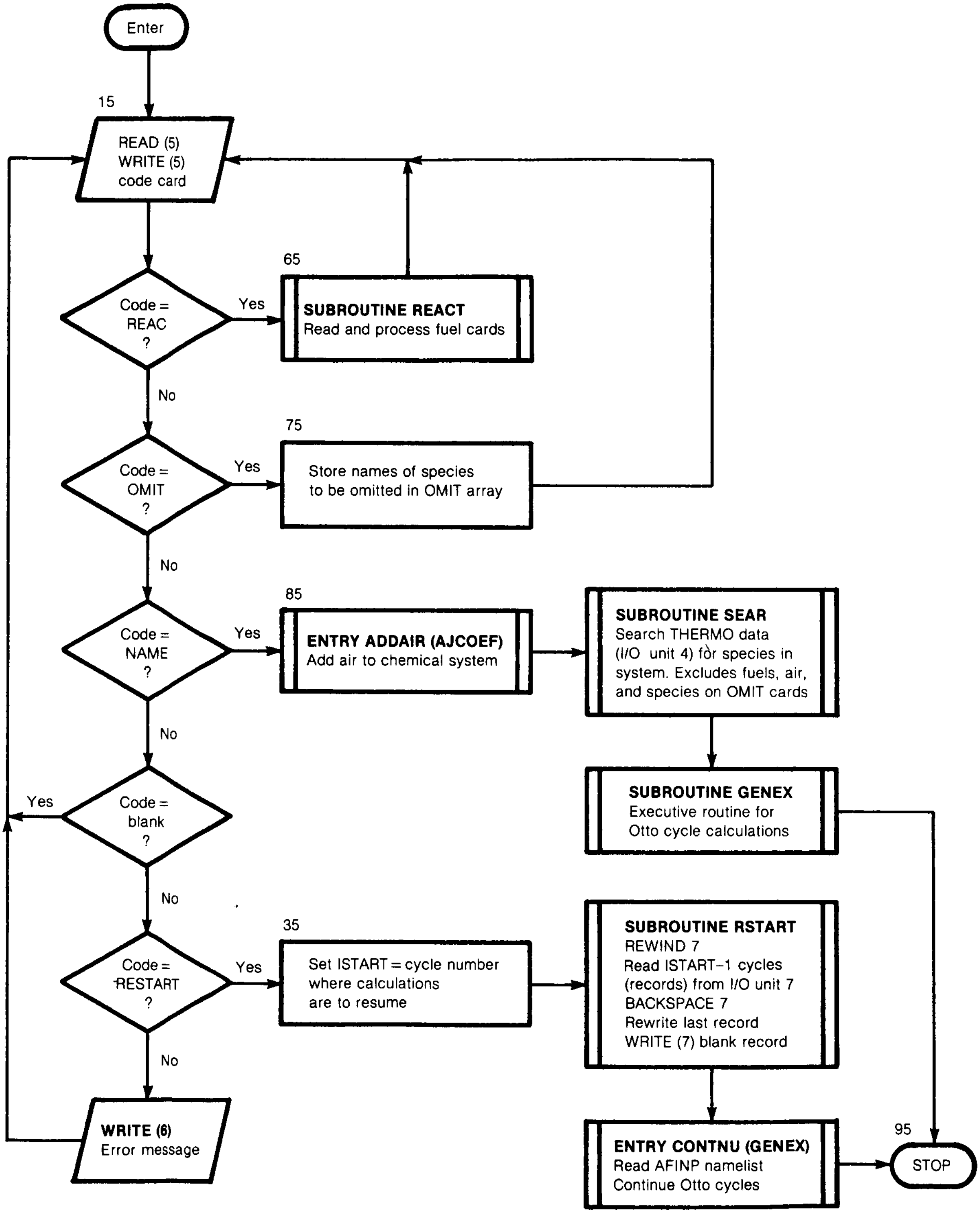
Appendix J contains flow diagrams of the main program and subroutine GENEX and a diagram showing the general flow between subroutines during combustion. The main program directs program flow according to whether it is an initial or restart run. Subroutine GENEX directs the cycle-to-cycle program flow for all levels. The purpose of the diagrams is to indicate general program flow, and only part of the actual code is included.

Numbers on the top left side of the boxes are program statement numbers. Called subroutines or entries are represented by boxes with double vertical lines. Entry names are followed by the subroutine name in parentheses. A brief description of what the routine does for the particular call is given within the box.

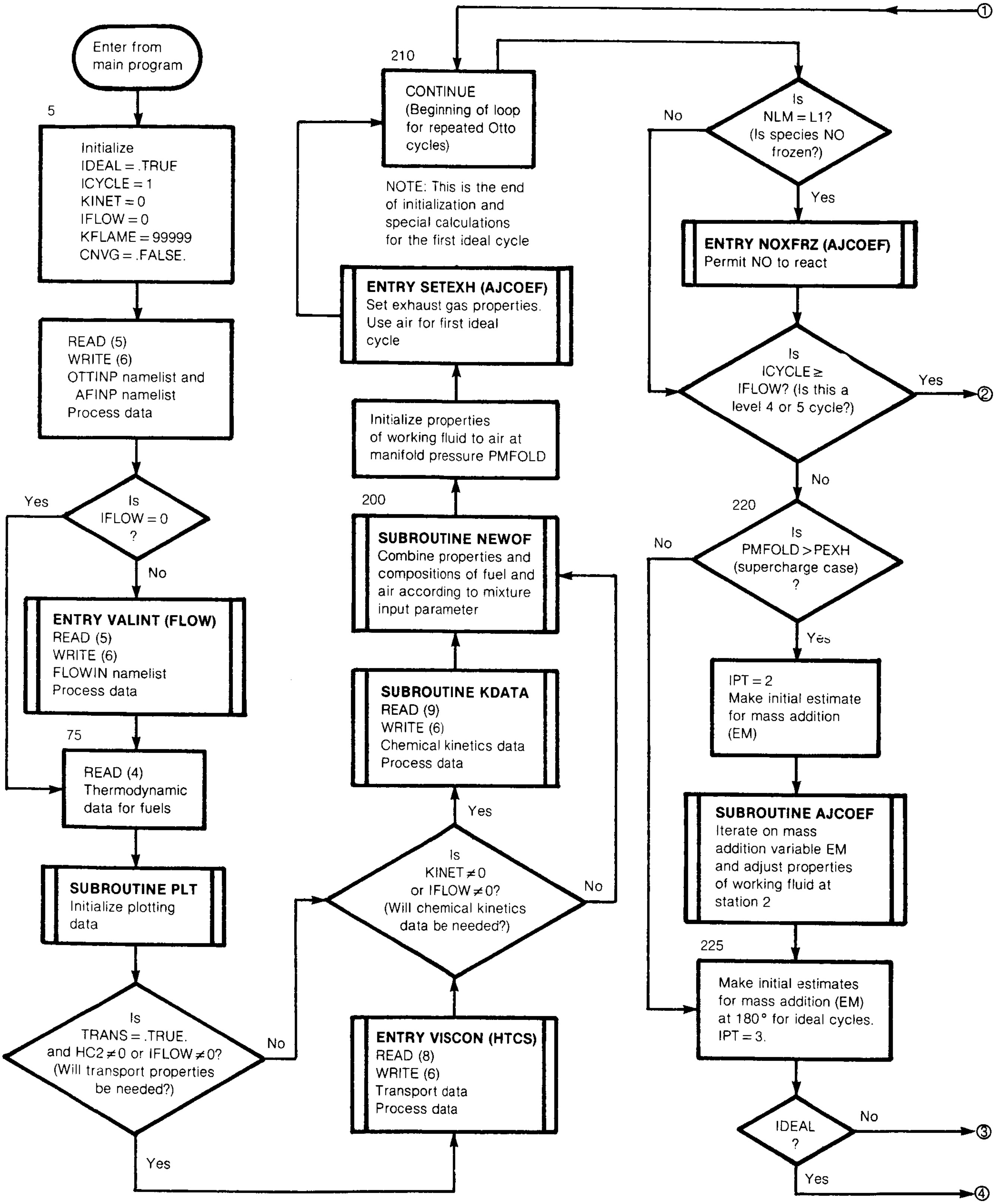
Cycle level and station numbers are referred to in many places throughout the diagrams. Figures 1 to 6 illustrate the definitions of these numbers. The variables EGR, HC2, IFLOW, KFLAME, KINET, PEXH, PMFOLD, RHUMID, and THBURN are defined in tables IV and V. Some other definitions are as follows:

CNVG	logical variable used for level 1 (ideal cycles); initialized to .FALSE. and set to .TRUE. when steady state is reached
EM	ratio of mass of fresh charge to mass of residual exhaust gas
FSTART	logical variable that is true only for level 4 or 5 calculations
ICYCLE	cycle number for either ideal or nonideal calculations
IDEAL	logical variable that is true for level 1 calculations
INT	integer that =3 for postcombustion calculations without flow (stations 5 and 6) =2 for burning calculations (stations 4 and 5) =1 for postcombustion calculations (stations 5 to 7) with flow =0 for no reactions and no flow (stations 1 to 4 and 7 to 8)
IPT	number of next station in cycle
L1	number of chemical components in system plus 1
NLM	number of components in chemical equilibrium calculations; equals number of chemical elements if species NO is allowed to react (i.e., not frozen); equals L1 if NO is frozen
NPROC	integer set to -1 if a case reaches normal completion; otherwise set to +1
TRANS	logical variable that is true for levels greater than 1

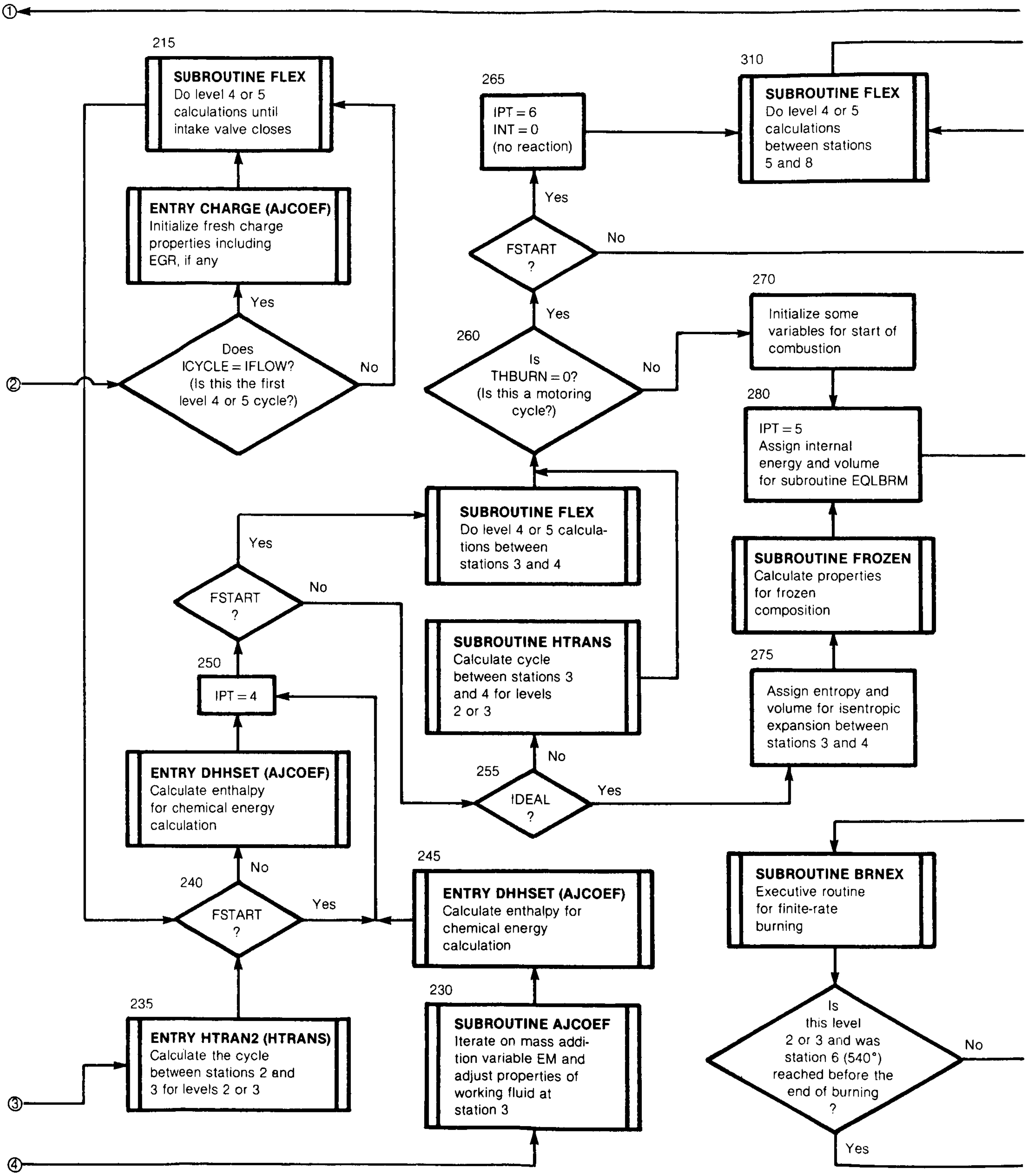
Main Program



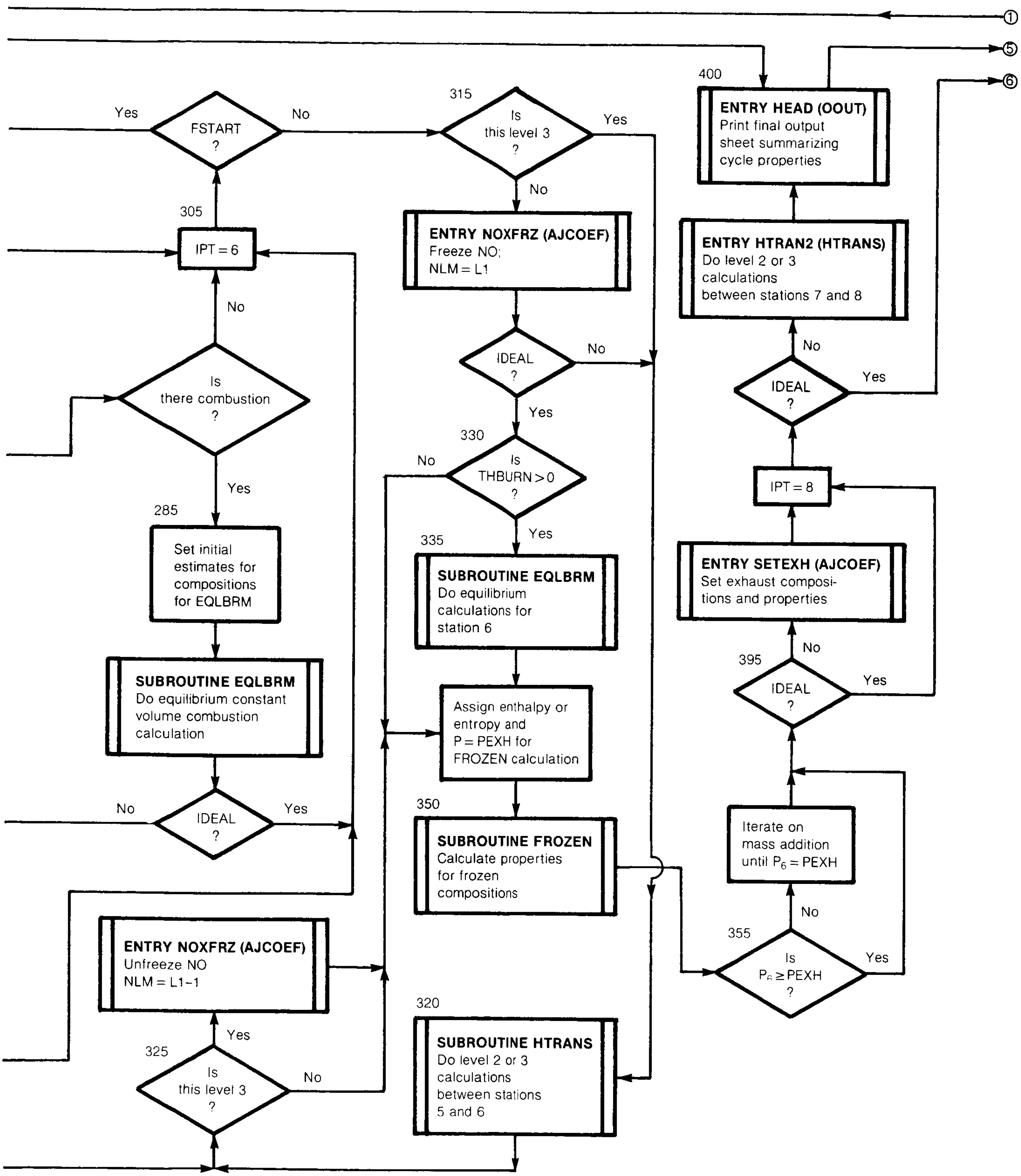
Subroutine GENEX



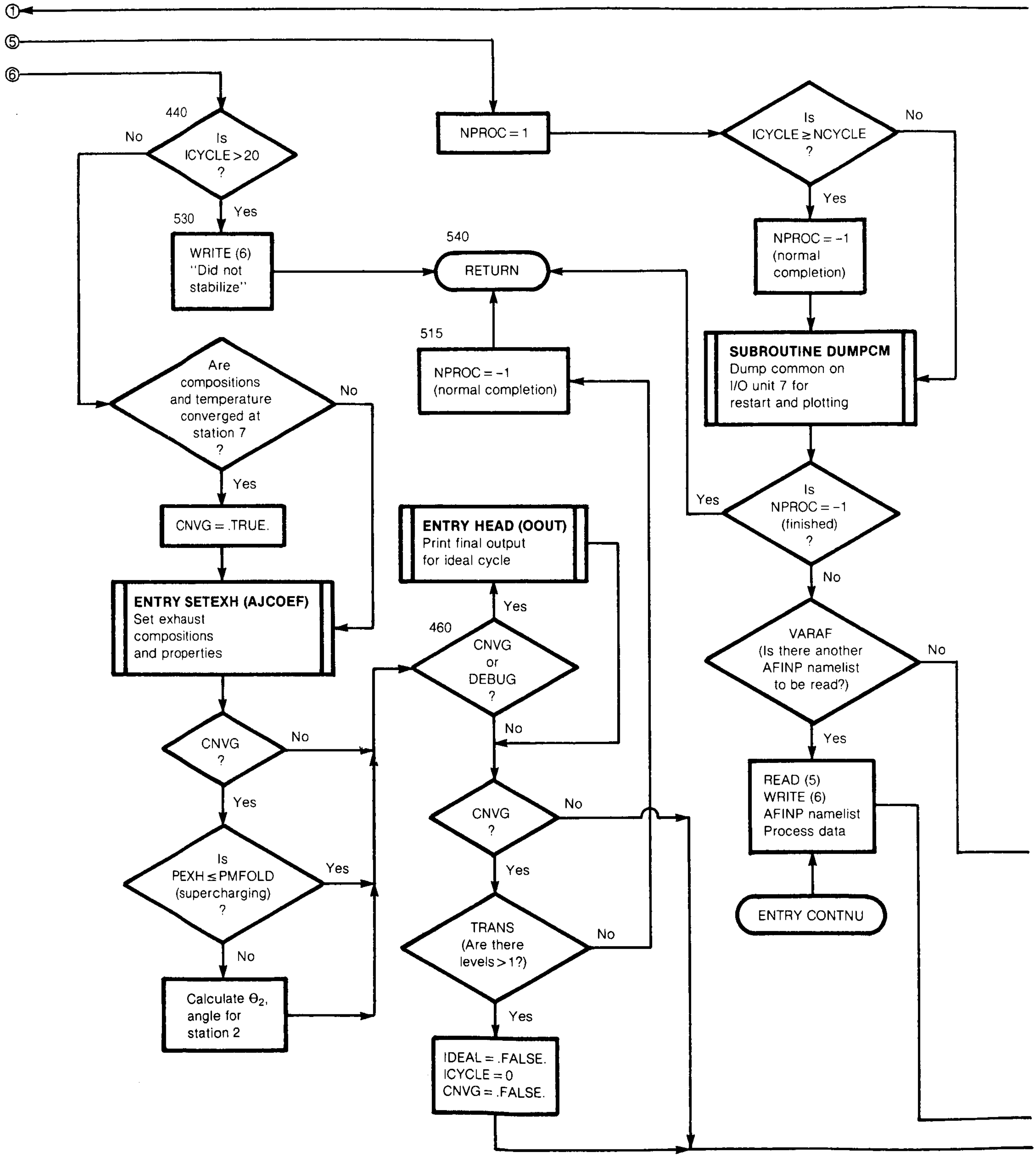
Subroutine GENEX (continued)



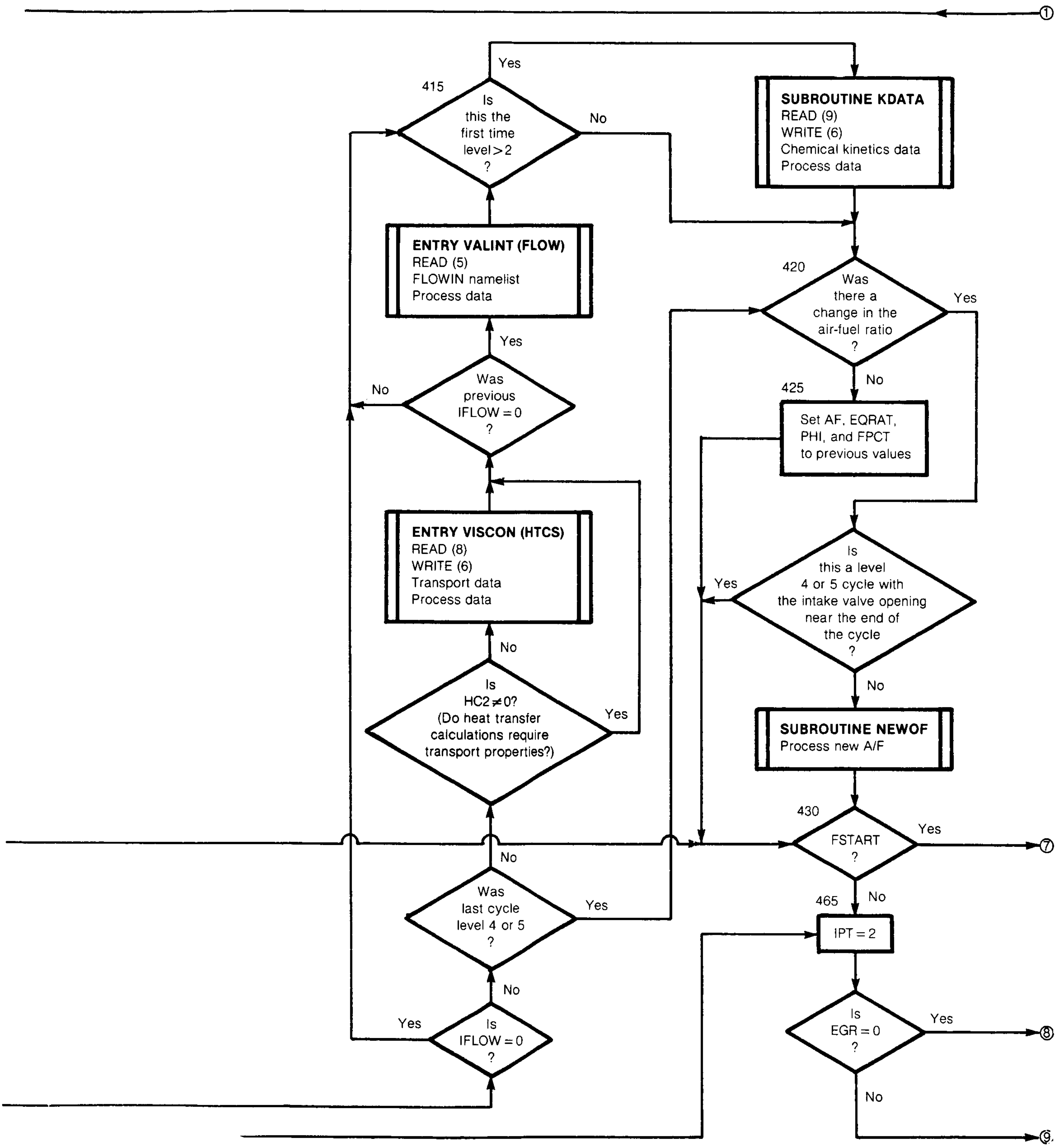
Subroutine GENEX (continued)



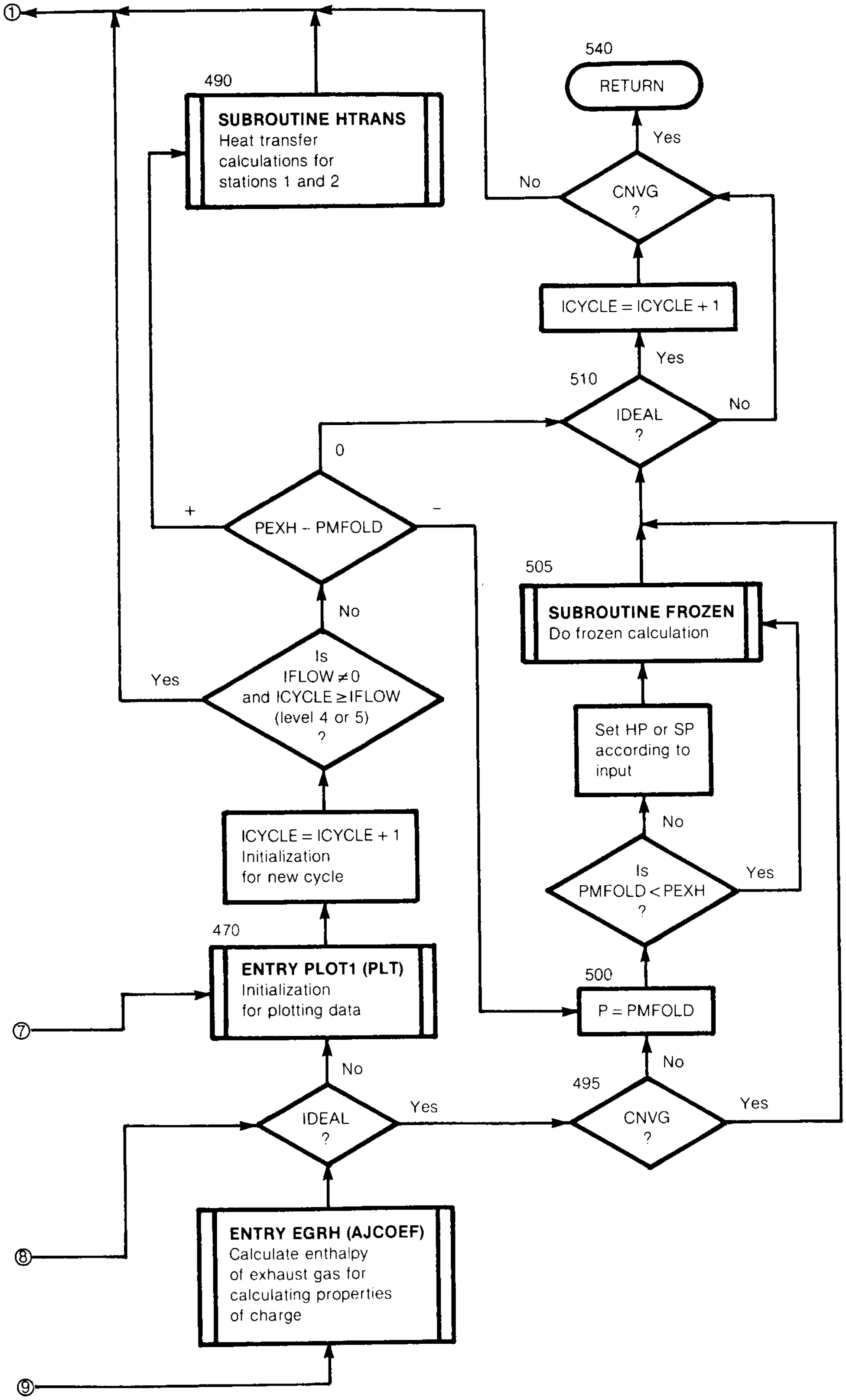
Subroutine GENEX (continued)



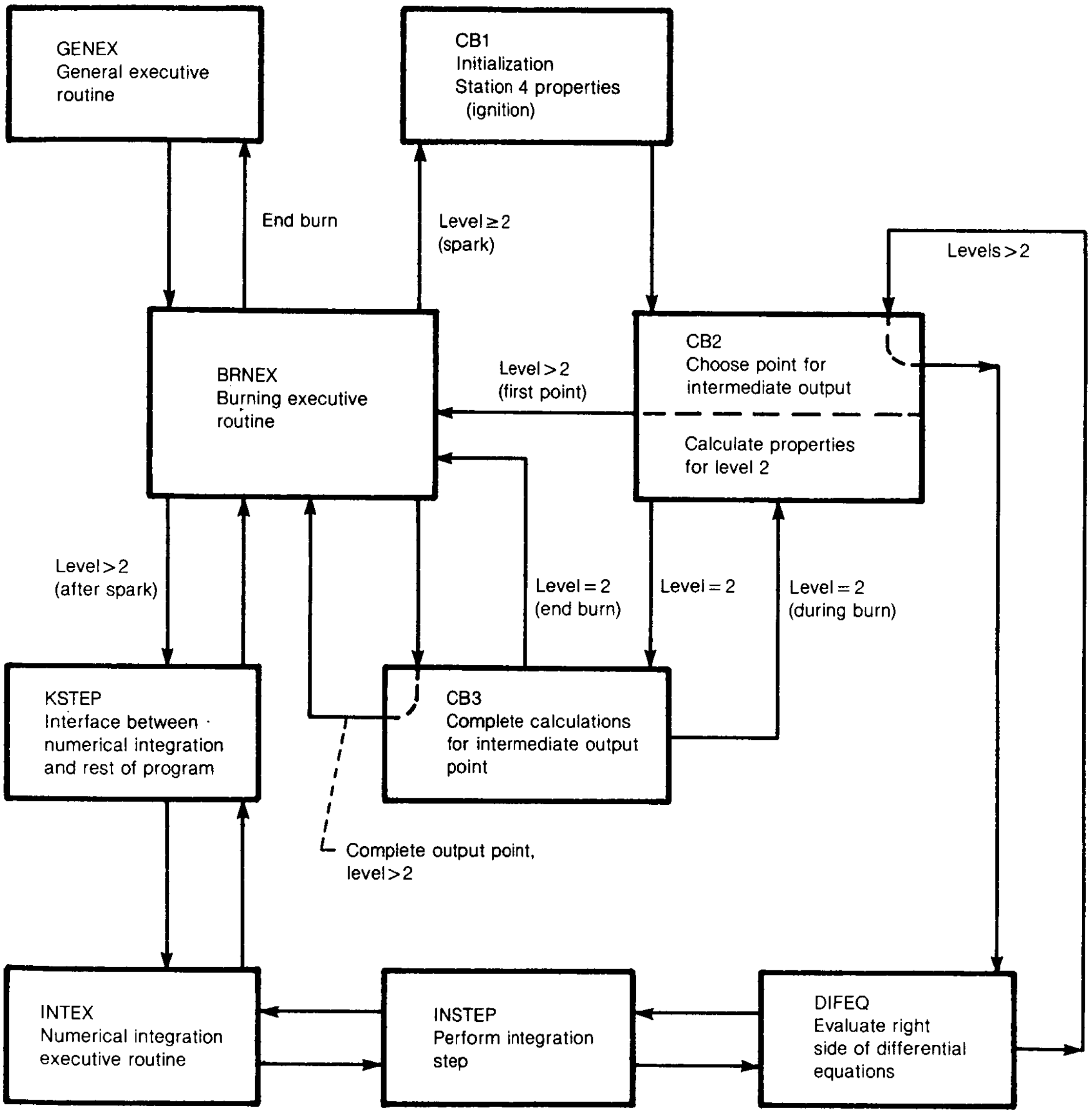
Subroutine GENEX (continued)



Subroutine GENEX (concluded)



Program Flow During Combustion



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16. Abstract

A flexible and computationally economical model of the internal combustion engine has been developed for use on large digital computer systems. It is based on a system of ordinary differential equations for cylinder-averaged properties. The computer program is capable of multicycle calculations, with some parameters varying from cycle to cycle, and has restart capabilities. It can accommodate a broad spectrum of reactants, permits changes in physical properties, and offers a wide selection of alternative modeling functions without any reprogramming. It readily adapts to the amount of information available in a particular case because the model is in fact a hierarchy of five models. The models range from a simple model requiring only thermodynamic properties to a complex model demanding full combustion kinetics, transport properties, and poppet valve flow characteristics. Among its many features the model includes heat transfer, valve timing, supercharging, motoring, finite burning rates, cycle-to-cycle variations in air-fuel ratio, humid air, residual and recirculated exhaust gas, and full combustion kinetics.

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