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MODELING THE COMPLETE OTTO CYCLE: PRELIMINARY VERSION

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ABSTRACT

A description is given of the equations and the computer program being developed to model the complete Otto cycle. The program incorporates such important features as: 1) heat transfer, 2) finite combustion rates, 3) complete chemical kinetics in the burned gas, 4) exhaust gas recirculation, and 5) manifold vacuum or supercharging. Changes in thermodynamic, kinetic and transport data as well as model parameters can be made without reprogramming. Preliminary calculations indicate that: 1) chemistry and heat transfer significantly affect composition and performance, 2) there seems to be a strong interaction among model parameters, and 3) a number of cycles must be calculated in order to obtain steady-state conditions.

THE INTERNAL COMBUSTION ENGINE has long been a source of frustration to those who would accurately and predictively model its behavior. It is not at all surprising that this should be the situation for the engine is inherently a very complex mechanical device. It is an open system with a movable boundary which exchanges both mass and energy with its environment, operates cyclicly over a broad range of temperatures and pressures, and contains matter which undergoes complex chemical transformations. This ubiquitous piece of hardware simultaneously embodies the principles of thermodynamics, chemical kinetics, transport phenomena, and fluid mechanics. Each separately is a challenge to the specialist; in concert they seem overwhelming. Yet, in spite of the difficulties, the modeler has pursued his objective impelled by a real need for the insight provided by model calculations.

The early attempts to make quantitative calculations were hampered on three fronts. There was a serious shortage of reliable physical data on thermodynamic, transport, and chemical rate properties. The computational capabilities were primitive by present standards. The numerical analysis that was necessary for effective computation had not yet been developed. To ameliorate the situation and permit at least rudimentary calculations, it was necessary for the early modelers to make gross simplifications. But in the intervening years, these three serious deficiencies have, in large measure, been corrected so that now 1) we have an ample and growing store of physical data, 2) there exist readily available large-scale computational facilities, and 3) many of the computational techniques are well understood. This growth in capability, if anything, has been exceeded by a growth of interest in understanding the workings of the internal combustion engine. The growth of interest has been catalyzed largely by federal pollution requirements and a national concern for the depletion of our petroleum resources. These factors have also been responsible for broadening the area of interest from only engine performance to include an interest in pollutant emissions.

At this juncture it seemed appropriate for us to reexamine the situation with respect to modeling the internal combustion engine. Our evaluation of the problem led us to several conclusions. First, we felt that any computer program should be independent of the particular physical data base used in the calculations. The reason for this is that although it is true that physical data are essential for the implementation of any mathematical model and do affect the results calculated by that model, they are not a part of the model itself but reflect the intrinsic properties of matter. Hence, it should be an easy task to incorporate additional or improved physical data as they become available and, further, the program's operation should not be adversely affected by data revision nor should data revision require any reprogramming. All too often we have seen apparently insignificant data changes produce unexpectedly large effects on the calculated results. Our approach permits the user to stop worrying about the effect of unnecessary data assumptions built into the model itself. At all times, the best and most complete data base is to be used in the calculations. The validity of this point of view is amply demonstrated by the success of our computer program for chemical equilibrium computations (1,2)* which has achieved a worldwide distribution. Second, the computer program should model the complete cycle, that is, it should model the induction and exhaust portions of the cycle as well as the compression and expansion phases of the cycle. Also it should be capable of repeatedly executing the cycle so that it can converge to the conditions that exist during the steady-state operation of the cycle. Third, the computer program should be capable of executing a full kinetic treatment of the chemistry rather than using a truncated reaction mechanism, such as the Zeldovich mechanism, and supplementing this with steady-state assumptions. Steady-state assumptions can only be justified _a posteriori_, that is, by a comparison of the results from a full kinetic treatment with those from the approximate treatment. Gelinas (3) made such a numerical comparison and concluded that the use of steady-state assumptions "is fraught with peril." Approximate chemistry may be adequate under some conditions and for some special purposes, as demonstrated by Annand (4), but to establish this adequacy one must be able to do the calculation with more nearly complete chemistry. Of course, multicycle calculations and complete kinetics demand efficient computation so as not to require an excessive amount of computer time. Fourth, there should be considerable flexibility in the choice of modeling functions and their parameters so that one can directly compare the results for different choices. Finally, fifth, the user should perceive the computer program as a black box for

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*Numbers in parentheses designate References at end of paper.

carrying out cycle calculations for his choices of physical data and modeling parameters, and he should not have to be concerned with the complexities of the computation. The results should be available not only in a convenient and easily digestible form, but also in a form which supplies as much detail as he could conceivably require.

At the time we began our work, we were not, and still are not, aware of any computer program which possessed all of these features which we deem to be so desirable. Many calculations were based on precalculated equilibrium properties which were then utilized with some interpolative scheme instead of calculating them as needed. Others made wholly unnecessary assumptions about thermodynamic data. Still others ignored heat transfer effects which strongly affect the temperature and which, in turn, could have a drastic influence on the composition through the temperature dependence of the thermodynamic, transport, and chemical rate data. Oftentimes only the closed system portion of the cycle was computed, based on estimated conditions at the start of the compression stroke. Generally, chemical kinetics was given short shrift either by ignoring it completely or else by drastically curtailing the number of reactions in the reaction mechanism and supplementing these with steady-state assumptions. Transport properties were totally ignored or were represented by the most gross approximations.

What are the prospects for developing a computer program to model the internal combustion engine which avoids those features which we find undesirable and incorporates those which we consider desirable? Clearly, we feel that it should be possible to accomplish the task, but also we realize that the foregoing considerations impose stringent constraints on the level of description that can be attempted in the modeling. Complete multicycle calculations and chemical kinetics separately, and certainly together, preclude modeling with partial differential equations because of the attendant vast requirements for computer time. Thus, the calculation must, of necessity, be based on a system of ordinary differential equations. This conclusion is reinforced by the stipulation that the calculations be independent of the particular data base, for then not only is there an increase in the bookkeeping overhead associated with the calculation but also one cannot take advantage of computational devices which might be dependent upon accidental characteristics of a given data base. To reap the potentially large benefits of broad applicability and convenience of use one must pay the price of increased computation time. This increased cost can be made quite modest by paying careful attention to numerical techniques.

On the following pages we shall briefly describe our attempt to achieve the objectives we have been discussing. We shall also illustrate the progress we have made up to this point with some typical calculations. However, neither our descriptions nor our illustrations should be regarded as our final words on the subject for we are continuing our development of the computer program and the analysis. Our ultimate goal is to use our computer program to predict engine behavior. To accomplish this we expect to use our program, together with engine data being generated at our laboratory, to determine suitable values for model parameters from experimental data as they become available.

GOVERNING DIFFERENTIAL EQUATIONS

For discussion purposes it is convenient to partition the Otto cycle into seven segments on a pressure-volume indicator diagram by eight points, two of which coincide. This can be seen in Fig. 1. Each segment corresponds to a different aspect of the cycle. The segment [1,2] represents the reduction of the residual exhaust gas pressure from the exhaust pressure to the manifold pressure. The induction of a fresh fuel-air-recirculated exhaust gas mixture and its mixing with the residual exhaust gases takes place on the segment [2,3]. The contents of the cylinder are compressed by the piston along segment [3,4] and combustion is initiated at the point labeled by 4. Combustion now continues on [4,5] where we have the coexistence of burned and unburned working fluids. Essentially all of the cylinder contents have been burned by the time point 5 has been reached and practically no unburned gas remains. The combustion products are then expanded along the segment [5,6]. At point 6 there is a sudden reduction of pressure to the exhaust pressure followed by the exhaust of the combustion products from the engine along segment [7,8]. A different system of differential equations is applicable, and is integrated, along each segment but there are always enough equations to determine the thermodynamic state of the working fluid and its composition. The specification of the state demands any two independent thermodynamic variables. During combustion, the burned and unburned gases each require two variables for a total of four.

We shall now simply give the equations which are the basis for our modeling of the seven segments of the cycle. The derivation and justification of these equations would take us too far afield and these aspects of the equations will not be discussed in this paper. Clearly the equations should be established with a minimum use of restrictive assumptions to achieve a maximum domain of applicability.

SEGMENT [1,2] AND SEGMENT [3,4] - Identical equations are used for segment [1,2] and segment [3,4]. The crankangle intervals corresponding to these segments are $0 = \theta_1 \leq \theta \leq \theta_2$ and $\pi = \theta_3 \leq \theta \leq \theta_4$, respectively.

$$\frac{du}{d\theta} = \frac{1}{M}\left[-p\,\frac{dV}{d\theta} - \frac{\dot{Q}}{\omega}\right] \tag{1}$$

$$\frac{dv}{d\theta} = v\left[\frac{1}{V}\,\frac{dV}{d\theta} - \frac{1}{M}\,\frac{dM}{d\theta}\right] \tag{2}$$

$$\frac{dn_\lambda}{d\theta} = 0 \qquad \lambda = 1,2,\ .\ .\ . \tag{3}$$

$$\frac{dM}{d\theta} = 0 \tag{4}$$

$$V = V(\theta) \tag{5}$$

$$M_2 = 0 \tag{6}$$

$$V_2 = 0 \tag{7}$$

SEGMENT [2,3] - The crankangle interval for this segment, which is the charge induction portion of the cycle, is $\theta_2 \leq \theta \leq \theta_3 = \pi$. The relevant equations are the following.

$$\frac{dh}{d\theta} = -\frac{\dot{Q}}{M\omega} + (h_0 - h)\,\frac{1}{M}\,\frac{dM}{d\theta} \tag{8}$$

$$\frac{dp}{d\theta} = 0, \qquad p(\theta_2) = p_M \tag{9}$$

$$\frac{dn_\lambda}{d\theta} = [n_\lambda(0) - n_\lambda]\,\frac{1}{M}\,\frac{dM}{d\theta} \tag{10}$$

$$\frac{dv}{d\theta} = v\left[\frac{1}{V}\,\frac{dV}{d\theta} - \frac{1}{M}\,\frac{dM}{d\theta}\right] \tag{11}$$

$$V = V(\theta) \tag{12}$$

$$\frac{dM_1}{d\theta} = 0 \tag{13}$$

The reactants comprising the fresh fuel-air mixture are initially presumed to be at a pressure p_F and are isentropically expanded to the pressure p_M prior to induction into the cylinder along [2,3].

SEGMENT [4,5]. This segment is the combustion phase of the cycle and the crankangle interval is $\theta_4 \leq \theta \leq \theta_5$.

$$\frac{du_1}{d\theta} = \frac{1}{M_1}\left[- p_1 \frac{dV_1}{d\theta} - \frac{\dot{Q}_1}{\omega} + (h_2 - u_1) \frac{dM_1}{d\theta}\right] \quad (14)$$

$$\frac{dv_1}{d\theta} = v_1\left[\frac{1}{V_1}\frac{dV_1}{d\theta} - \frac{1}{M_1}\frac{dM_1}{d\theta}\right] \quad (15)$$

$$\frac{dn_\lambda^{(1)}}{d\theta} = \frac{R_\lambda}{\rho_1\omega} + \left[n_\lambda^{(eq)} - n_\lambda^{(1)}\right]\frac{1}{M_1}\frac{dM_1}{d\theta}$$

$$\lambda = 1, 2, \ldots \quad (16)$$

$$\frac{du_2}{d\theta} = \frac{1}{M_2}\left[- p_2 \frac{dV_2}{d\theta} - \frac{\dot{Q}_2}{\omega} + (h_2 - u_2) \frac{dM_2}{d\theta}\right] \quad (17)$$

$$\frac{dv_2}{d\theta} = v_2\left[\frac{1}{V_2}\frac{dV_2}{d\theta} - \frac{1}{M_2}\frac{dM_2}{d\theta}\right] \quad (18)$$

$$\frac{dn_\lambda^{(2)}}{d\theta} = 0 \qquad \lambda = 1, 2, \ldots \quad (19)$$

$$p_1 = p_2 \quad (20)$$

$$v_1M_1 + v_2M_2 = V \quad (21)$$

$$M_1 + M_2 = M \quad (22)$$

$$\frac{dM}{d\theta} = 0 \quad (23)$$

$$M_1 = M_1(\theta) \quad (24)$$

If the products of combustion are to be in chemical equilibrium along [4,5], then this assumption is used to replace the differential equations for $n_\lambda^{(1)}$.

SEGMENT [5,6] - The crank angle interval for the post-combustion phase of the cycle is $\theta_5 \leq \theta \leq \theta_6 = 3\pi$. The following equations are used to calculate the working fluid properties for this segment.

$$\frac{du}{d\theta} = \frac{1}{M}\left[- p \frac{dV}{d\theta} - \frac{\dot{Q}}{\omega}\right] \quad (25)$$

$$\frac{dv}{d\theta} = v\left[\frac{1}{V}\frac{dV}{d\theta} - \frac{1}{M}\frac{dM}{d\theta}\right] \quad (26)$$

$$\frac{dn_\lambda}{d\theta} = \frac{R_\lambda}{\rho\omega} \qquad \lambda = 1, 2, \ldots \quad (27)$$

$$\frac{dM}{d\theta} = 0 \quad (28)$$

$$V = V(\theta) \quad (29)$$

$$M_2 = 0 \quad (30)$$

If the products are to be in chemical equilibrium along [5,6] then, as for [4,5], this assumption is used to replace the differential equations for n_λ, except for NO which is as assumed to be nonreacting.

SEGMENT [6,7] - The sudden reduction of the pressure to exhaust pressure is calculated from the following equations for $\theta_6 = \theta_7 = 3\pi$.

$$n_\lambda(\theta_7) - n_\lambda(\theta_6) = 0 \quad (31)$$

$$s(\theta_7) - s(\theta_6) = 0 \quad (32)$$

$$p(\theta_7) - p_E = 0 \quad (33)$$

$$v(\theta_7)M(\theta_7) - v(\theta_6)M(\theta_6) = 0 \quad (34)$$

SEGMENT [7,8] - This segment of the cycle corresponds to the exhaust stroke for which $3\pi = \theta_7 \leq \theta \leq \theta_8 = 4\pi$.

$$\frac{dh}{d\theta} = - \frac{\dot{q}}{M\omega} \quad (35)$$

$$\frac{dp}{d\theta} = 0, \qquad p(\theta_7) = p_E \quad (36)$$

$$\frac{dn_\lambda}{d\theta} = 0 \qquad \lambda = 1, 2, \ldots \quad (37)$$

$$v(\theta) = V(\theta)/M(\theta) \quad (38)$$

$$V = V(\theta) \quad (39)$$

In essence, these equations imply that the Otto cycle is an open system only for the segments [2,3], [6,7], and [7,8]. Chemical reactions occur only in the burned gases and there only along [4,5], and [5,6]. The reaction rates are determined either by chemical kinetic data or by equilibrium thermodynamics. For the latter case NO is assumed to be nonreacting in the post combustion segment [5,6]. When chemical kinetics governs the combustion process, it is assumed that the unburned gas passes through the flame front and is injected into the burned gas at the equilibrium composition corresponding to the enthalpy and pressure of the unburned gas. Heat and work can be exchanged between the working fluid and its environment at all points of the cycle. There is no heat transferred between the burned and unburned working fluid, and both are at the same pressure but not the same temperature.

The preceding equations are the ones we have selected as the governing equations for the seven segments of the Otto cycle, but any attempt to implement them in the given form would certainly lead to serious numerical difficulties. These equations have been converted to numerically useful forms; however, the details of the transformations would entail the discussion of a substantial amount of analysis. For that reason this topic will not be discussed here.

MODELING FUNCTIONS - The systems of equations we have been discussing are complete in the sense that their solutions can be used to completely characterize the Otto cycle at the level of description that we have chosen (ordinary differential equations). The equations themselves are, however, still incompletely specified because they contain functions, called modeling functions, which remain to be defined. These functions include the heat loss functions $\dot{Q}$, $\dot{Q}_1$, and $\dot{Q}_2$, the mass burning function M_1, the volume function V, and the species rate of production functions R_λ. It is important to realize that while there are sometimes conventional choices which are made for some of these functions, it is by no means certain that the conventional choices are the "best" choices. It is certainly possible, and in fact likely, that there is no uniquely "best" choice. The ultimate criteria for a good choice are adequate agreement with experiment and extrapolation adequacy. Nonetheless, to perform any calculations one must make a choice. We must make some specific choices because we wish to present the results of some typical calculations within the framework of our general approach in order to illustrate the versatility and computational costs and also to demonstrate some parametric effects. We do not wish to attach any particular significance to the ad hoc choices we make for these calculations. We might well make different choices for subsequent calculations. The following equations give our choices of the modeling functions for this paper.

$$V(\theta) = V_c\Big\{1 + (r - 1)[1 - \cos\theta + (1 - \sqrt{1 - \varepsilon^2 \sin^2\theta})/\varepsilon]\Big/2\Big\} \qquad (40)$$

$$\varepsilon = L/2\ell \qquad (41)$$

$$M_1(\theta)\begin{cases} = M_1(\theta_4) + \dfrac{M - M_1(\theta_4)}{2\left[1 + \left(\dfrac{\pi\theta_\tau}{\theta_f - \theta_4}\right)^2\right]}\Bigg\{1 - \cos\pi\left(\dfrac{\theta - \theta_4}{\theta_f - \theta_4}\right) \\ \qquad - \left(\dfrac{\pi\theta_\tau}{\theta_f - \theta_4}\right)\sin\pi\left(\dfrac{\theta - \theta_4}{\theta_f - \theta_4}\right) + \left(\dfrac{\pi\theta_\tau}{\theta_f - \theta_4}\right)^2 (1 - \exp[-(\theta - \theta_4)/\theta_\tau])\Bigg\} & \theta_4 \le \theta \le \theta_f \\ = M_1(\theta_f) + [M - M_1(\theta_f)]\{1 - \exp[-(\theta - \theta_f)/\theta_\tau]\} & \theta_f \le \theta_5 \end{cases} \qquad (42)$$

$$\dot{Q} = \bar{h}A(T - T_w) \qquad (43)$$

$$\dot{Q}_1 = \bar{h}A_1(T_1 - T_w) \qquad (44)$$

$$\dot{Q}_2 = \bar{h}A_2(T_2 - T_w) \qquad (45)$$

$$A = A_c + 2(r - 1)V_c[1 - \cos\theta + (1 - \sqrt{1 - \varepsilon^2 \sin^2\theta})/\varepsilon]/B \qquad (46)$$

$$A_1 = AM_1/M \qquad (47)$$

$$A_2 = AM_2/M \qquad (48)$$

$$\bar{h}\begin{cases} = c_1(L\omega/\pi)^{1/3}(pT)^{1/2} & \text{Eichelberg} \quad (49) \\ = c_2(k/B)(BL\omega\rho/\pi\mu)^{0.7} + c_3(T^4 - T_w^4)/(T - T_w) & \text{Annand} \quad (50) \\ = c_4(k/B)(c_p\mu/k)^{0.4}(BL\omega\rho/\pi\mu)^{0.8} & \text{Dittus-Boelter} \quad (51) \end{cases}$$

Equation (40) for $V(\theta)$ is just the usual volume-crankangle equation used for the four stroke piston engine. Equation (42) for $M_1(\theta)$ is taken from (5). For $\theta_\tau = 0$ it reduces to the mass burning expression of Blumberg and Kummer (6) and for $\theta_\tau \neq 0$ it is the extension of their formula to incorporate the relaxation effects of Blizard and Keck (7). The heat loss formulas are the conventional ones involving the heat-transfer coefficient. The expressions for A_1 and A_2 were motivated by the knowledge that the separation of the working fluid into burned and unburned fractions by the flame front is sufficiently indistinct that A_1 and A_2 cannot be determined precisely. Further, they possess the desirable property that as the mass approaches zero, so does the heat transfer surface. We assume the usual rate expressions of chemical kinetics for R_λ. If $c_1 = 1.25\times10^{-5}$, c_2 in the interval (0.35, 0.8), $c_3 = 1.025\times10^{-13}$, and $c_4 = 0.023$, then the formulas for the heat transfer coefficient, in cal-cm^{-2}-sec^{-1}-K^{-1}, are the correlations of Eichelberg (8), Annand (9), and Dittus-Boelter. The latter is a correlation for heat transfer accompanied by the turbulent flow of a fluid in a pipe. Each of the heat transfer correlations has features not possessed by the other two. The Eichelberg form is the one most commonly used and has no composition dependence. The Annand form has a radiation term and depends on composition through the thermal conductivity. The Dittus-Boelter form depends on composition through both the thermal conductivity and the shear viscosity.

To conclude the discussion of modeling functions, we wish to point out that many modeling functions, like the formulas for the heat transfer coefficient, often contain parameters which are determined from experimental data by a comparison with calculated results. But since the calculated results can be strongly affected by the governing equations and by the physical data, one should realize that the parameters may have to be redetermined as the ability to calculate improves. That is, experimentally determined parameters may be model sensitive.

PHYSICAL DATA

An extremely important part of any modeling computer program is the physical data base which is used in the calculations. To model the internal combustion engine with the equations of the previous section we require thermodynamic data for each of the chemical species which appear in the working fluid. For each species, we must know the heat capacity, the enthalpy, and the entropy. All of the necessary thermodynamic computations are performed with our own equilibrium computations program (2). Hence, the thermodynamic data are just those which we supply with that program and these are supplemented by some additional data for the fuels which are needed for the calculations to be reported in this paper.

The transport properties of the working fluid appear in two of the three formulas for heat transfer coefficients. The shear viscosity and thermal conductivity data for the pure species were based on experimental measurements where possible and, when necessary, this was augmented with theoretically estimated properties. Except for the thermal conductivity of carbon dioxide, the transport properties came from (10 to 13). The thermal conductivity of carbon dioxide was obtained from a smoothed curve through experimental data from 16 references published from 1950 to 1968. The mixture properties were calculated from the data for the pure species with the mixture formula for viscosity suggested by Bromley and Wilke (14) and the mixture formula of Lindsay and Bromley (15) for thermal conductivity. The mixture thermal conductivity formula was modestly altered so as to make use of information contained in the shear viscosity data.

The chemical kinetics data consisted of the rate constants and equilibrium constants for the 19 forward reactions listed in Table 1. This table contains only homogeneous reactions and we will neglect all wall reactions. It should be noted that four of the listed reactions involve third bodies and so each of these reactions corresponds to 14 forward reactions, one for each possible third body. The rate constant data for the individual forward reactions came from (16) for all reactions except reaction 13 and reaction 19. The rate constants for these two reactions came from (17) and (18), respectively. The equilibrium constant data used to compute the rate constants for the backward reactions from the forward rates came from the same thermodynamic data mentioned previously. The net production rates R_λ were calculated by the method described by Bittker and Scullin (19) and we used the appropriate portions of their computer program to carry out the calculations.

SOME CALCULATED RESULTS AND THEIR IMPLICATIONS

THE STANDARD PROBLEM - Our purpose in presenting the results of some numerical calculations is 1) to display the capabilities of the present version of our Otto cycle computer program, 2) to make an assessment of the validity of equilibrium thermodynamics during combustion as an approximation for chemical reaction effects, 3) to try to make a judgment about the degree of interaction of model parameters, 4) to determine the sequence and number of cycles which should be calculated to determine steady state conditions and 5) to make some estimate of the computation times involved. We do not intend to carry out a detailed parametric study at this time because we feel that too many of the model parameters given in the literature are so poorly estimated that such a calculation would be premature.

Our computer program for modeling the Otto cycle is already very versatile in its present stage of development. It can accommodate so many parameters that it would be a herculean task to illustrate the effects of each one. Since our purpose is only to make some general observations about the calculations, we shall arbitrarily fix a number of parameters at what might be considered reasonable values. The assigned values are shown in Table 2. These values, together with $p_F = p_E = 760$ mm Hg, $p_M = 250$ mm Hg, a stoichiometric air-fuel ratio, no recirculated exhaust gas, $\tau = 0$, and a frequency of 500 revolutions per minute will define a standard set of conditions for all comparison purposes. The heat transfer parameters c_2 and c_4 were chosen so that the heat loss was identical for all three heat transfer correlations for the standard conditions and a particular cycle in the sequence of cycle calculations.

The discussion of the calculated results will be facilitated if we first introduce some terminology associated with the sequence of cycle calculations executed by the computer program. To reach steady state conditions with the least amount of computer time usage, it is desirable to begin the calculation with the most highly idealized model and sequentially introduce departures from the ideal. The greater the idealization the simpler the calculation and, hence, the shorter the computation time. Thus, the computation begins with a set of n_I ideal cycle calculations corresponding to equilibrium combustion at constant volume and zero heat transfer during the cycle. The actual number of ideal cycles computed is the number required to achieve steady state operation, defined by the condition that the cycle to cycle change in exhaust gas temperature at point 7, $T(\theta_7)$, is less than 1 K. These ideal cycles are then followed by n_E cycles which are somewhat less idealized and include the effects of heat transfer and a finite combustion rate. The composition of the burned gas is still governed by equilibrium thermodynamics. These cycles in turn are followed by n_K cycles where chemical kinetics is used to determine the burned gas composition in place of equilibrium thermodynamics. The nonnegative integers n_E and n_K are arbitrary and are limited only by the available computation time. A given calculation can then be labeled by the triplet of integers (n_I, n_E, n_K). The heat transfer parameters c_2 and c_4 were chosen so as to give identical heat losses for the calculation (n_I, 3, 0) of the standard problem, that is, at the conclusion of the third equilibrium cycle.

Some calculated results for the standard problem, using the Eichelberg form of the heat transfer correlation, are shown in graphical form as Figs. 2 to 12. These figures are computer generated plots which are pretty much self-explanatory and are the results of the (3, 3, 0) calculations. That is, these results are for the third equilibrium combustion cycle which was preceded by three ideal cycles. Each figure is labeled by the date of the calculation, a case number and a cycle number. The first digit of the case number identifies the form of the heat transfer correlation (1 = Eichelberg, 2 = Dittus-Boelter, 3 = Annand) and the next two digits give the revolutions per minute in hundreds of revolutions. The cycle number is the number of cycles calculated after the steady state ideal cycle. The term "cylinder average" used in Figs. 7 and 8 refers to an average over the burned and unburned gases.

From these figures, one can see that the values of all properties agree at $\theta = 0^o$ and $\theta = 720^o$ and hence, these figures correspond to a steady state where combustion is controlled by thermodynamics. The curves in Figs. 2, 3, 4, and 9 possess discontinuities at $\theta = 540^o$ which occur because of the sudden reduction of the pressure to p_E. Figures 9 to 11 each have two curves. One curve is either the heat or the work and the other is 100 times its rate of change with respect to crankangle. On the boundaries of the Otto cycle segments, that is, at the distinguished points of Fig. 1, the rate of change is the actual derivative at the initial point of the segment. At all other points the rate of change is the mean rate of change obtained by averaging the rate of change over intervals determined by the computer program. The discontinuity in the heat loss rate at the end of combustion (point 5) arises for this reason and occurs because of the rapid change in the heat loss rate in this portion of the cycle.

CHEMICAL KINETICS EFFECTS - What is the effect of replacing equilibrium thermodynamics with chemical kinetics and calculating two additional cycles for the same problem, that is, doing the calculation (3, 3, 2)? For this particular calculation, using the Eichelberg heat transfer correlation, there is essentially no change in temperature, pressure, work, and heat loss. There are, however, changes in the concentrations of the pollutants carbon monoxide and nitric oxide. These are displayed in Figs. 13 to 16 for the calculation (3, 3, 2). Again, because the values at $\theta = 0^\circ$ and $\theta = 720^\circ$ are equal, these results correspond to a new steady-state where combustion is controlled by chemical kinetics. A comparison of these figures with those given as Figs. 5 to 8 shows that a considerable difference exists between pollutant concentrations calculated on the basis of thermodynamic equilibrium and those calculated on the basis of chemical kinetics. Chemical kinetics calculates higher concentrations for both pollutants. The differences in results between these two assumptions are further emphasized by the data given in Table 3. It shows the dependence of the calculated results on the cycle number and the heat transfer correlation for the standard problem. Here we again see evidence that a steady state has been achieved in the standard problem for (3, 3, 0) for the four kinds of heat loss calculations and all three heat transfer correlations do indeed give the same heat loss on the third equilibrium combustion cycle. Two additional kinetic combustion cycles suffice for the attainment of a new steady-state for the quantities listed in Table 3. It is obvious from the data in Table 3 that heat losses cannot be ignored because they profoundly alter the calculated results as can be seen by comparing the zero heat transfer calculation with the other three calculations.

A new and somewhat surprising feature appears in Table 3. While there is very little interaction between the chemistry and the Eichelberg heat transfer correlation, chemistry does have an appreciable effect on the heat losses calculated by the other two heat transfer correlations. Also changes were produced in the indicated mean effective pressure, the indicated specific fuel consumption as well as the temperatures and pressures. This points up the model sensitivity of heat transfer parameters and should cause one to question the correctness of heat transfer parameters determined from the combination of experimental data and model calculations which ignore chemical kinetics. But, to the best of our knowledge, all calculations prior to those reported here have not had the combination of a general heat transfer correlation with complete chemical kinetics. Thus it follows that those correlations that already exist in the literature must be used with considerable caution. Further, the strength of the interaction between chemistry and heat transfer should cause one to suspect, and be wary of, strong interactions among other parameters. For this reason, it seems probable that very few model parameters can be isolated for experimental determination. It is more likely that most model parameters must be evaluated simultaneously from all of the available experimental data.

Table 3 leads us to two other important conclusions. First, the $(n_I, 3, 2)$ calculation seems to be adequate for obtaining an estimate of the true steady-state conditions. Second, the estimation of the concentration of the pollutants CO and NO_x by equilibrium combustion and frozen NO in the post combustion region may be in serious error. This latter point is corroborated by the data in Table 4 which shows the amount of NO_x, expressed as grams of NO_x per kilogram of burned gas, calculated by the two methods discussed in this paper as well as the values calculated if the NO were frozen at the peak temperature. The first part of the table shows the dependence on frequency and the choice of heat transfer correlation while the second part shows the dependence on equivalence ratio for the Eichelberg heat transfer correlation at a fixed frequency of 3500 revolutions per minute. From Table 4 we see that freezing NO at the end of combustion is superior to freezing it at the peak temperature as a device for estimating NO_x; however, neither technique gives a particularly good approximation to the kinetically calculated values.

Exhaust gas recirculation has been used as a method for reducing the emission of NO_x but it should, and does, affect the concentrations of other species in the exhaust. For case 135 the specific productions of NO_x and CO in g/kw-sec are 4.62×10^{-3} and 3.13×10^{-3}, respectively, for (3, 3, 0) and 4.40×10^{-3} and 3.12×10^{-3} for (3, 3, 2). The addition of a sufficient amount of recirculated exhaust gas so that it represents 15% of the working fluid by mass (case 13515) changes these values to 2.53×10^{-3} and 1.57×10^{-3} for (3, 3, 0) and 1.93×10^{-3} and 1.68×10^{-3} for (3, 3, 2). Thus for both equilibrium combustion and kinetic combustion the recirculation of exhaust gas significantly reduces the production of NO_x and CO.

One of the most difficult pollutants to handle in a model of the internal combustion engine is the unburned hydrocarbons. Zeleznik (5) suggested that the relaxation approach of Blizard and Keck (7) might offer an approach to the problem. To see if unburned hydrocarbons could be made to appear in the exhaust we repeated case 135 but set $\tau = 0.0009$. The result was that for this case, designated 13509, 1.9 parts per million hydrocarbon appeared in the exhaust. Hence, this is indeed a means for introducing hydrocarbon into the exhaust. The only question is whether or not one can determine the parameter τ so as to reproduce experimental unburned hydrocarbon data. This can only be answered after an extensive analysis of calculated results and experimental data.

The concentrations of CO and NO generally behave qualitatively as shown in Figs. 5 to 8 and Figs. 13 to 16; there are, of course, significant quantitative differences. But we have also seen cases where the qualitative behavior differs appreciably from what we have shown. As an example of a different kind of behavior, we show in Figs. 17 and 18 the concentrations of CO and NO in the burned gas of the calculation (3, 3, 2) of case 13509 and case 13515, respectively. Here the carbon monoxide decreases initially before it begins its rise to a maximum. The nitric oxide rises to, and then remains at, its maximum value.

DETERMINATION OF HEAT TRANSFER PARAMETERS - What are the prospects for determining parameters in heat transfer correlations from experimental data? The prospects would be excellent if the calculated results were strongly dependent upon these model parameters through some externally controllable parameters such as frequency and air-fuel ratio. We have already seen from Tables 3 and 4 that the composition is moderately dependent on both the form of the heat transfer correlation and the frequency and is strongly dependent on equivalence ratio. Hence data on pollutant concentrations in the exhaust might be of some help in evaluating heat transfer parameters. What about the frequency dependence of heat loss and indicated work and its relationship to the heat transfer correlation? This is shown in the first part of Table 5 where we give the frequency dependence of the heat loss and the indicated work for the three correlations used in this paper at the steady-states for equilibrium and kinetic combustion. From these data we see that the frequency dependence of the heat loss and work is greatest when the calculation is made with the Eichelberg heat transfer correlation and weakest for the calculations made with the Dittus-Boelter correlation. But in any event, the frequency dependence of the calculated results is sufficiently different for the three correlations that it should be possible to use experimental heat loss and work data to choose from among various correlations. The information derived from the frequency dependence could be augmented by exploring the dependence of the heat loss and work on the air-fuel ratio. The kind of variation predicted with the Eichelberg correlation is shown in the second part of Table 5 and it seems reasonable that the results calculated with the other correlations should be affected even more strongly because of their greater sensitivity to the chemistry.

The Annand form for the heat transfer coefficient is the only correlation which tries to make an allowance for radiation. Is this T^4 term likely to contribute significantly to the heat loss? Since heat loss per cycle decreases as the revolutions per minute increases, the gas temperatures should be the highest at 5000 rpm. Hence, the radiation contribution should approach its maximum value under these conditions. We, therefore, repeated the calculation for case 350 but eliminated radiation effects by setting the constant c_3 to zero. This decreased the heat loss by about 1.5% and increased the work by about 0.3% for both kinetic and equilibrium combustion chemistry. Thus, the effect of radiation seems to be quite small and probably cannot be determined from experimental data with any real accuracy.

COMPUTATION TIMES - It is very difficult to make any precise statements about computation times since they are so variable not only from one machine to another but also from one installation of the same machine to another. All our computations were carried out on an IBM 360/67 duplex with the TSS/360 operating system. This computer has virtually unlimited storage capacity but is generally considered to be a relatively slow machine by current standards. The computation times we will cite are for an unoptimized program used on this machine and we could have reduced the times by about 10 to 15% with relatively little effort.

The ideal cycles typically take about 2.5 seconds of computer time. Cycles in which combustion is computed by equilibrium thermodynamics take about 1 to 2 minutes of computer time. Those computed with the Eichelberg heat transfer correlation are closer to one minute while the other two correlations require times closer to 2 minutes. The cycles for which the composition is determined by chemical kinetics exhibit the greatest variability in the usage of computer time and also somewhat longer computation times. These times span the range from about 1.5 minutes to about 4 minutes. For comparable conditions the calculations using the Eichelberg heat transfer correlation require the least time. Generally, the computation time decreases as the frequency increases and it tends to decrease as one moves away from stoichiometric conditions.

It is gratifying to find that the computation times for a full kinetic cycle calculation are not drastically different from the computation times for an equilibrium cycle calculation. The increased computation cost is quite modest. In fact, the cost is so modest that it becomes difficult to justify the use of approximate kinetics, such as the Zeldovich mechanism coupled with steady-state assumptions, because the sole purpose of these approximations is to simplify the computation and thus reduce the computation times. The increased cost is certainly warranted since it dispels any doubts one would have about results based on the use of steady-state assumptions.

CONCLUSIONS

Based on our calculations it is possible to draw a number of conclusions about modeling the complete internal combustion engine cycle. First, and most important, it is feasible and practical to model the complete cycle with ordinary differential equations with both expanded finite rate chemistry during the combustion and post-combustion phases and heat transfer. Second, chemistry and heat transfer significantly affect not only composition but also measures of cycle performance such as work. Third, there appears to be a sufficiently strong interaction among model parameters so as to preclude the isolation of individual parameters for experimental determination. It may be necessary to evaluate a number of parameters simultaneously. Fourth, in the sequence of cycle calculations discussed here, it seems that one can adequately determine steady-state conditions with the calculation $(n_I,3,2)$. Fifth, the estimation of pollutant concentrations by neglecting finite rate chemistry or heat transfer is questionable.

ACKNOWLEDGEMENT

We wish to thank Helen Hu for writing the computer plotting routines that we used to generate Figs. 2 to 18.

SYMBOLS

A	surface area for heat transfer
A_c	surface area of combustion chamber
B	bore
c_p	heat capacity at constant pressure
h	enthalpy per unit mass
h_0	enthalpy per unit mass for fresh charge
$\bar{h}$	heat transfer coefficient (gas side)
k	thermal conductivity
L	stroke
ℓ	connecting rod length
M	mass of the working fluid
n_λ	moles of species λ per unit mass
$n_\lambda(0)$	moles species λ per unit mass for fresh charge
$n_\lambda^{(eq)}$	equilibrium composition from combustion of unburned gas at h_2, p_2
p	pressure
p_E	exhaust pressure
p_F	fuel pressure
p_M	manifold pressure
$\dot{Q}$	heat loss rate
R_λ	volumetric production rate of species
r	compression ratio
s	entropy per unit mass
T	temperature
T_w	effective wall temperature for heat transfer
u	internal energy per unit mass
V	volume

V_c	volume of combustion chamber
v	volume per unit mass
θ	crankangle
θ_i	$i = 1, 2, \ldots, 8$ crankangles corresponding to the 8 distinguished points on the indicator diagram given in Fig. 1
θ_τ	$\omega\tau$
θ_f	crankangle for which all unburned gas has passed through the flame front
μ	shear viscosity
ρ	mass density
τ	relaxation time for combustion
ω	angular frequency

SUBSCRIPTS AND SUPERSCRIPTS

1	burned gas
2	unburned gas

REFERENCES

1. F. J. Zeleznik and S. Gordon, "Calculation of Complex Chemical Equilibria." Ind. Eng. Chem., Vol. 60 (1968), No. 6, p. 27.

2. S. Gordon and B. J. McBride, Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations." NASA SP-273, Interim Revision, 1976.

3. R. J. Gelinas, "Stiff Systems of Kinetic Equations - A Practitioner's View." J. Comp. Phys., Vol. 9 (1972), No. 2, p. 222.

4. W. J. D. Annand, "Effects of Simplifying Kinetic Assumptions in Calculating Nitric Oxide Formation in Spark-Ignition Engines." Proc. Instn. Mech. Eng., Vol. 188 41/74 (1974), p. 431.

5. F. J. Zeleznik, "Combustion Modeling in Internal Combustion Engines." Comb. Sci. Tech., Vol. 12, No. 4-6, p. 159.

6. P. Blumberg and J. T. Kummer, "Prediction of NO Formation in Spark-Ignited Engines - An Analysis of Methods of Control." Comb. Sci. Tech., Vol. 4 (1971) No. 2, p. 73.

7. N. G. Blizard and J. C. Keck, "Experimental and Theoretical Investigation of Turbu-

lent Burning Model for Internal Combustion Engines." SAE Paper 740191 presented at the Automotive Engineering Congress, Detroit, Feb. 1974.

8. G. Eichelberg, "Some New Investigations on Old Combustion Problems." Engineering (London), vol. 148 (1939), p. 603.

9. W. J. D. Annand, "Heat Transfer in the Cylinders of Reciprocating Internal Combustion Engines." Proc. Instn. Mech. Engrs., Vol. 177 (1963), No. 36, p. 973.

10. H. J. M. Hanley, "The Viscosity and Thermal Conductivity Coefficients of Dilute Argon, Krypton, and Xenon." Phys. and Chem. Ref. Data, Vol. 2 (1973), No. 3, p. 619.

11. H. J. M. Hanley and J. F. Ely, "The Viscosity and Thermal Conductivity Coefficients of Dilute Nitrogen and Oxygen." J. Phys. and Chem. Ref. Data, Vol. 2 (1973), No. 4, p. 735.

12. G. C. Maitland and B. E. Smith, "Critical Reassessment of Viscosities of 11 Common Gases." J. Chem. and Eng. Data, Vol. 17 (1972), No. 2, p. 150.

13. R. A. Svehla and B. J. McBride, "Fortran IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems. NASA TN D-7056, 1973.

14. L. A. Bromley and C. R. Wilke, "Viscosity Behavior of Gases." Ind. Eng. Chem., Vol. 43 (1951), No. 7, p. 1641.

15. A. L. Lindsay and L. A. Bromley, "Thermal Conductivity of Gas Mixtures." Ind. Eng. Chem., Vol. 42 (1950), No. 8, p. 1508.

16. R. F. Hampson, Jr. and D. Garvin, eds., "Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry." NBS Tech Note 866, 1975.

17. W. Hack, K. Hoyermann, and H. Gg. Wagner, "The Reaction $NO + HO_2 \rightarrow NO_2 + OH$ with $OH + H_2O_2 \rightarrow HO_2 + H_2O$ as an HO_2 Source." Int. J. Chem. Kinetics, Symposium No. 1 (1975), p. 329.

18. D. L. Baulch, D. D. Drysdale and A. C. Lloyd, "Critical Evaluation of Rate Data for Homogeneous Gas-Phase Reactions of Interest in High Temperature Systems." University, Leeds (1968).

19. D. A. Bittker and V. J. Scullin, "General Chemical Kinetics Computer Program for Static and Flow Reactions, with Application to Combustion and Shock-Tube Kinetics. NASA TN D-6586, 1972.

Table 1 - Summary of Reaction Mechanism and Rate Constants

k for Kinetically Controlled Combustion

Reaction number	Reaction	Third body, M	$k = AT^n e^{-E/RT}$ cm^3/mole-sec A	n	E
1	$N + OH \rightarrow NO + H$		4×10^{13}	0	0
2	$M + O + O \rightarrow O_2 + M$	O_2	1.38×10^{18}	-1	340
3	$N + NO \rightarrow N_2 + O$		1.6×10^{13}	0	0
4	$N + O_2 \rightarrow NO + O$		6.6×10^{9}	1	6 260
5	$O + NO_2 \rightarrow NO + O_2$		1×10^{13}	0	596
6	$M + NO + O \rightarrow NO_2 + M$	O_2	1.1×10^{15}	0	-1 870
7	$H + O_2 \rightarrow OH + O$		2.2×10^{14}	0	16 800
8	$O + H_2 \rightarrow OH + H$		1.8×10^{10}	1	8 900
9	$H + HO_2 \rightarrow OH + OH$		2.5×10^{14}	0	1 890
10	$OH + HO_2 \rightarrow H_2O + O_2$		5×10^{13}	0	994
11	$O + HO_2 \rightarrow OH + O_2$		4.8×10^{13}	0	994
12	$M + H + O_2 \rightarrow HO_2 + M$	Ar	2.4×10^{15}	0	-576
13	$HO_2 + NO \rightarrow OH + NO_2$		1.2×10^{13}	0	2 390
14	$H + NO_2 \rightarrow NO + OH$		3.5×10^{14}	0	1 470
15	$O + H_2O \rightarrow OH + OH$		6.6×10^{13}	0	18 370
16	$H_2 + OH \rightarrow H_2O + H$		2.2×10^{13}	0	5 150
17	$CO + OH \rightarrow CO_2 + H$		3.1×10^{11}	0	596
18	$M + H + OH \rightarrow H_2O + M$	Ar	1.4×10^{22}	-2	0
19	$O + CO_2 \rightarrow CO + O_2$		1.9×10^{13}	0	54 150

Third body efficiencies are 1.0 except for the following:

Reaction	$M = O_2$	$M = H_2O$	$M = CO_2$	$M = N_2$	$M = CO$
12	2	32.5	7.5	2	2
18	1.6	20.0	7.5	1.6	1.6

Table 2 - Some Parameter Assignments

Fuel composition, mass percent		Combustion parameters
n-Octane	42	$\theta_4 = 350^\circ$
Toluene	38	$\theta_f - \theta_4 = 30^\circ$
Benzene	18	$M_1(\theta_5)/M(\pi) = 0.9999$
1-Octene	2	$\tau = 0$

Air composition, mole percent		Heat transfer parameters
Nitrogen	78.0881	$c_1 = 1.2504 \times 10^{-5}$
Oxygen	20.9495	$c_2 = 0.3872$
Argon	0.9324	$c_3 = 1.0253 \times 10^{-13}$
Carbon dioxide	0.03	$c_4 = 0.73$

Engine and operating parameters

$B = 10.922$ cm (4.3 in.)
$L = 10.312$ cm (4.06 in.)
$\ell = 17.145$ cm (6.75 in.)
$r = 10.5$
$A_c = 129.032\ \text{cm}^2$ (20.0 in.^2)
$p(\theta_2) = p_M$
$T_w = 360$ K

Table 3 - The Effect of Heat Transfer on Calculated Results at 500 Rev/min

Cycle*	Average exhaust temp., K	NO_x	CO, ppm	Heat loss, Joules	IMEP, atm	ISFC, g/kW-sec
			Zero Heat Transfer			
1	1229.4	11 640	0	0	6.4898	0.04867
2	1470.7	8 210	2380	0	5.9411	.05152
3	1469.9	7 880	6170	0	5.7902	.05210
4	1472.4	6 159	5012	0	5.8042	.05135
5	1471.9	6 150	5004	0	5.8062	.05137
6	1471.8	6 150	5004	0	5.8063	.05137
7	1485.8	3 833	3266	0	5.8320	.05114
8	1485.7	3 835	3264	0	5.8260	.05117
			Eichelberg Heat Transfer Correlation			
4	798.0	4 197	1800	604.83	4.8163	0.06521
5	783.6	3 199	1288	560.11	4.7310	.06392
6	783.1	3 170	1274	558.89	4.7289	.06390
7	781.6	3 460	2376	558.38	4.7182	.06405
8	781.9	3 461	2372	558.24	4.7197	.06403
			Dittus-Boelter Heat Transfer Correlation			
4	798.0	4 053	1788	593.37	4.5843	0.06600
5	772.9	3 000	1202	560.68	4.5479	.06478
6	771.6	2 950	1174	558.88	4.5426	.06475
7	724.8	3 453	2380	590.24	4.4621	.06592
8	723.1	3 401	2347	588.12	4.4576	.06583
			Annand Heat Transfer Correlation			
4	784.5	4 340	1870	599.75	4.7386	0.06487
5	763.6	3 205	1264	560.60	4.6685	.06365
6	762.7	3 160	1241	558.94	4.6637	.06364
7	683.2	3 476	2416	625.25	4.4300	.06699
8	681.3	3 388	2352	620.72	4.4235	.06682

*Cycles 1-3 Instantaneous burning and equilibrium chemistry
Cycles 4-6 Finite rate burning and equilibrium chemistry
Cycles 7-8 Finite rate burning and finite rate chemistry

Table 4 - Predicted NO_x (g NO_x/kg burned gas) by Different Methods

	Kinetic combustion			Equilibrium combustion			Peak temperature		
Rev/min	Eichel-berg	Dittus-Boelter	Annand	Eichel-berg	Dittus-Boelter	Annand	Eichel-berg	Dittus-Boelter	Annand
500	3.55	3.49	3.48	3.25	3.03	3.24	4.65	4.53	4.60
1500	4.45	3.94	4.08	4.51	3.54	4.02	5.55	4.86	5.21
3500	4.91	4.11	4.35	5.68	3.89	4.49	6.67	5.20	5.53
5000	5.02	4.16	4.43	5.37	4.02	4.65	6.24	5.31	5.71

Eichelberg Heat Transfer Correlation, 3500 Revolutions per Minute

Equivalence ratio	Kinetic combustion	Equilibrium combustion	Peak temperature
0.8	7.50	7.97	9.12
.9	7.11	7.43	8.41
1.0	4.91	5.68	6.67
1.1	2.29	2.45	3.12
1.2	.86	1.17	1.79

Table 5 - The Interaction of Chemistry and Heat Transfer

A. Frequency Dependence of Heat Loss and Indicated Work in Joules

	Equilibrium combustion			Kinetic combustion		
Rev/min	Eichelberg	Dittus-Boelter	Annand	Eichelberg	Dittus-Boelter	Annand
			Heat loss			
500	558.89	558.88	558.94	558.24	588.12	620.72
1500	366.15	491.12	447.72	366.13	520.15	512.93
3500	243.27	439.60	369.83	243.15	467.25	431.89
5000	201.37	418.44	339.58	200.66	444.73	399.62
			Indicated work			
500	462.92	444.69	456.54	462.02	436.36	433.03
1500	524.50	472.39	497.95	524.02	465.74	478.90
3500	548.68	489.97	519.70	547.80	484.30	503.86
5000	554.77	496.52	526.74	553.64	491.12	512.02

B. Equivalence Ratio Dependence of Heat Loss and Indicated Work in Joules for the Eichelberg Heat Transfer Correlation at 3500 Rev/Min

Equivalence ratio	Equilibrium combustion	Kinetic combustion
	Heat Loss	
0.8	185.04	185.09
.9	216.66	216.66
1.0	243.27	243.15
1.1	233.01	233.11
1.2	220.67	219.95
	Indicated work	
0.8	468.11	468.54
.9	512.49	512.60
1.0	548.68	547.80
1.1	550.73	551.33
1.2	547.17	547.65

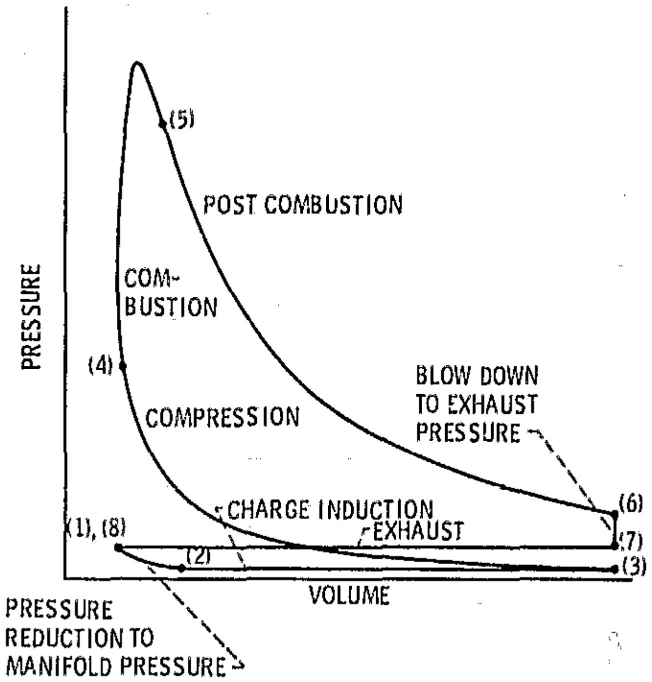

Figure 1. - Otto cycle indicator diagram.

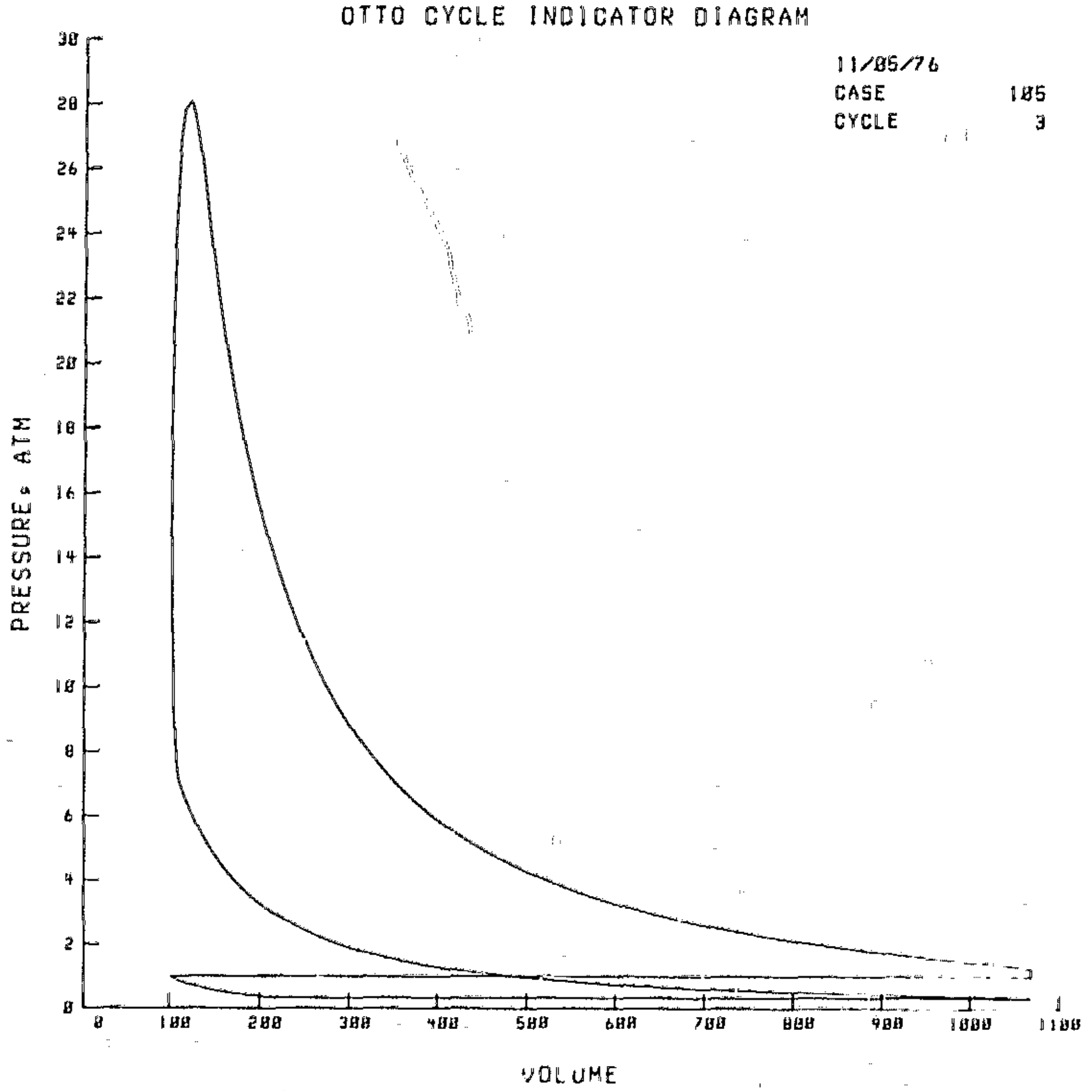

Fig. 2 - Calculated indicator diagram

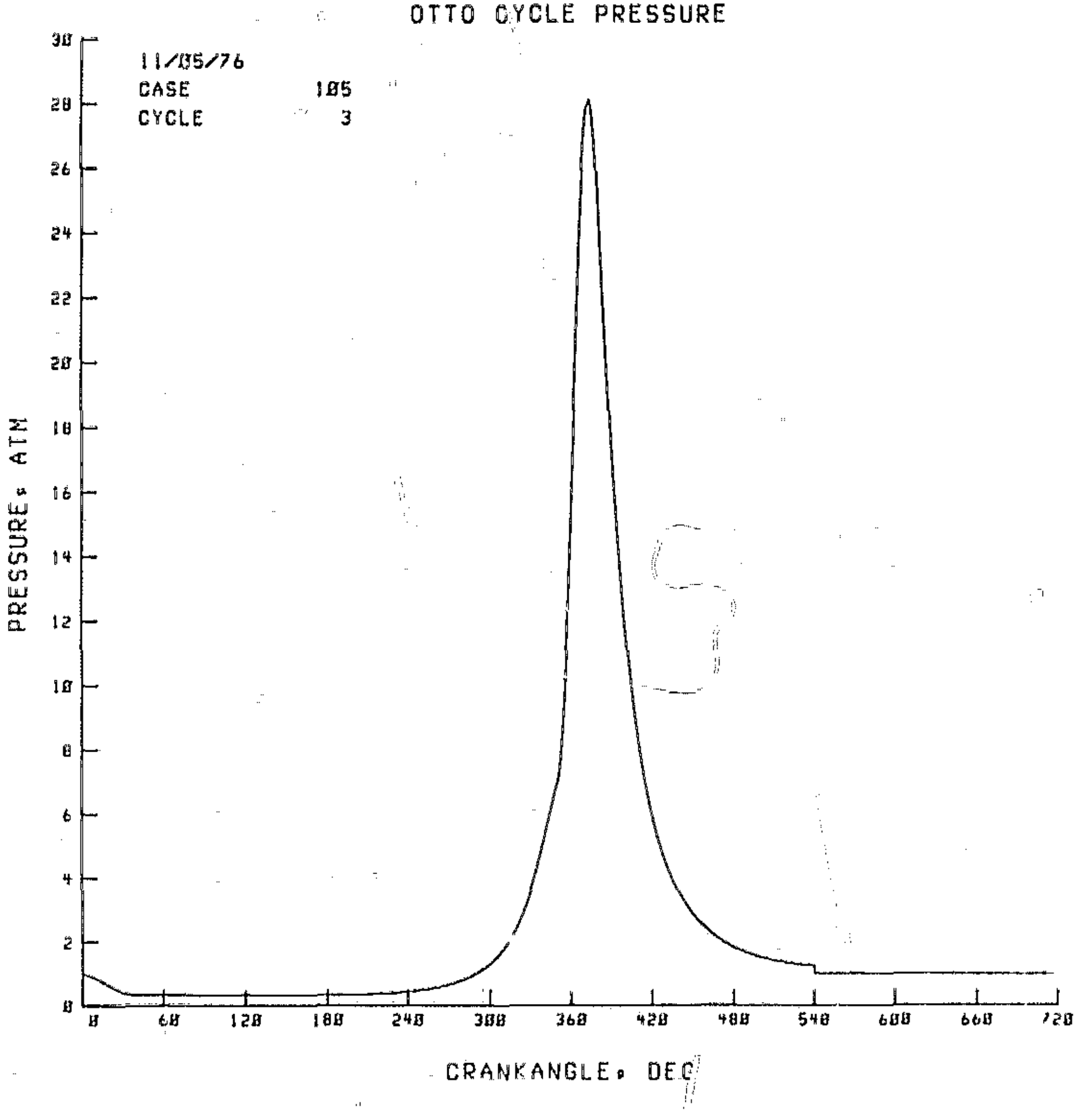

Fig. 3 - Calculated cylinder pressure

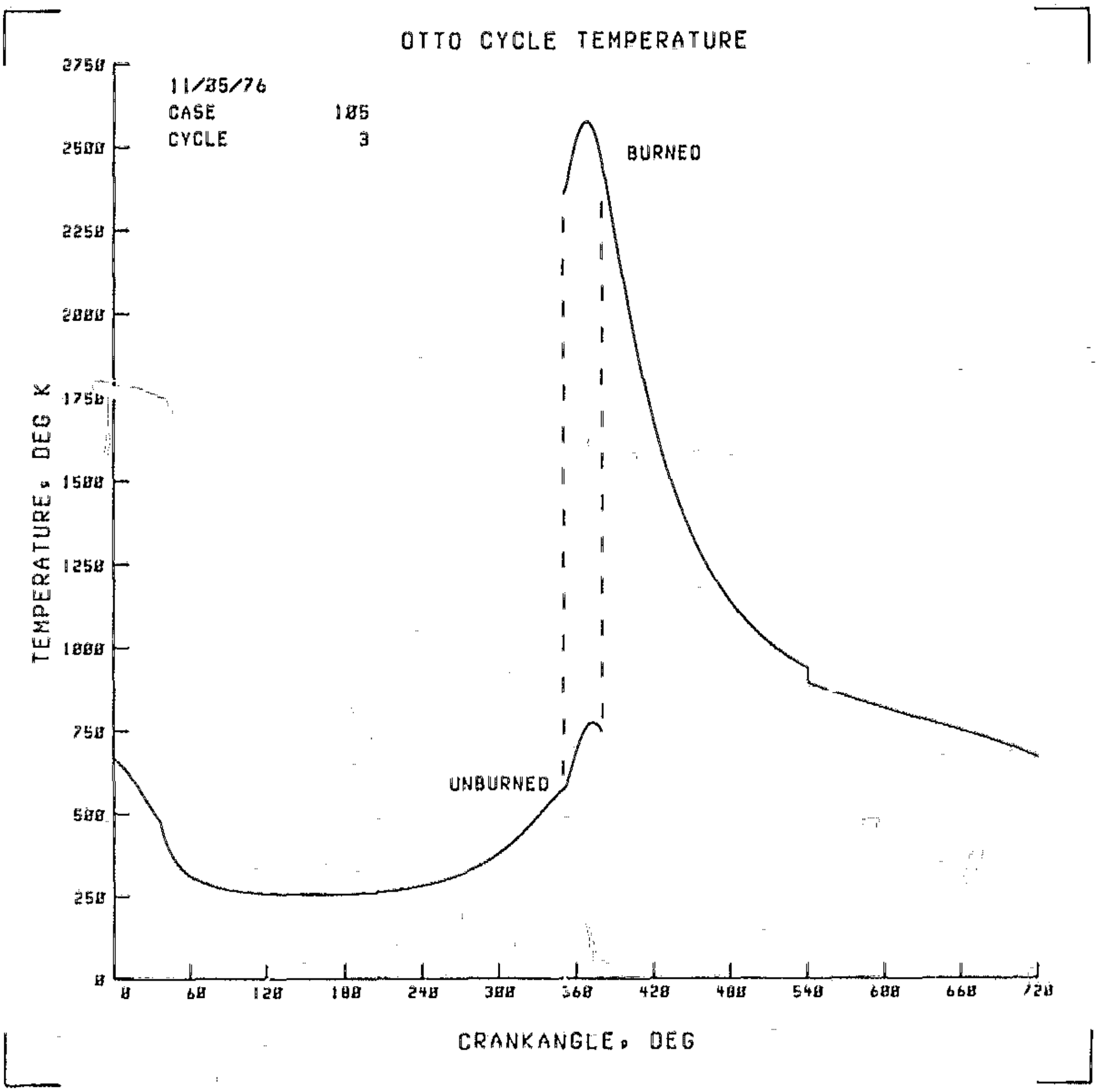

Fig. 4 - Calculated burned and unburned gas temperatures

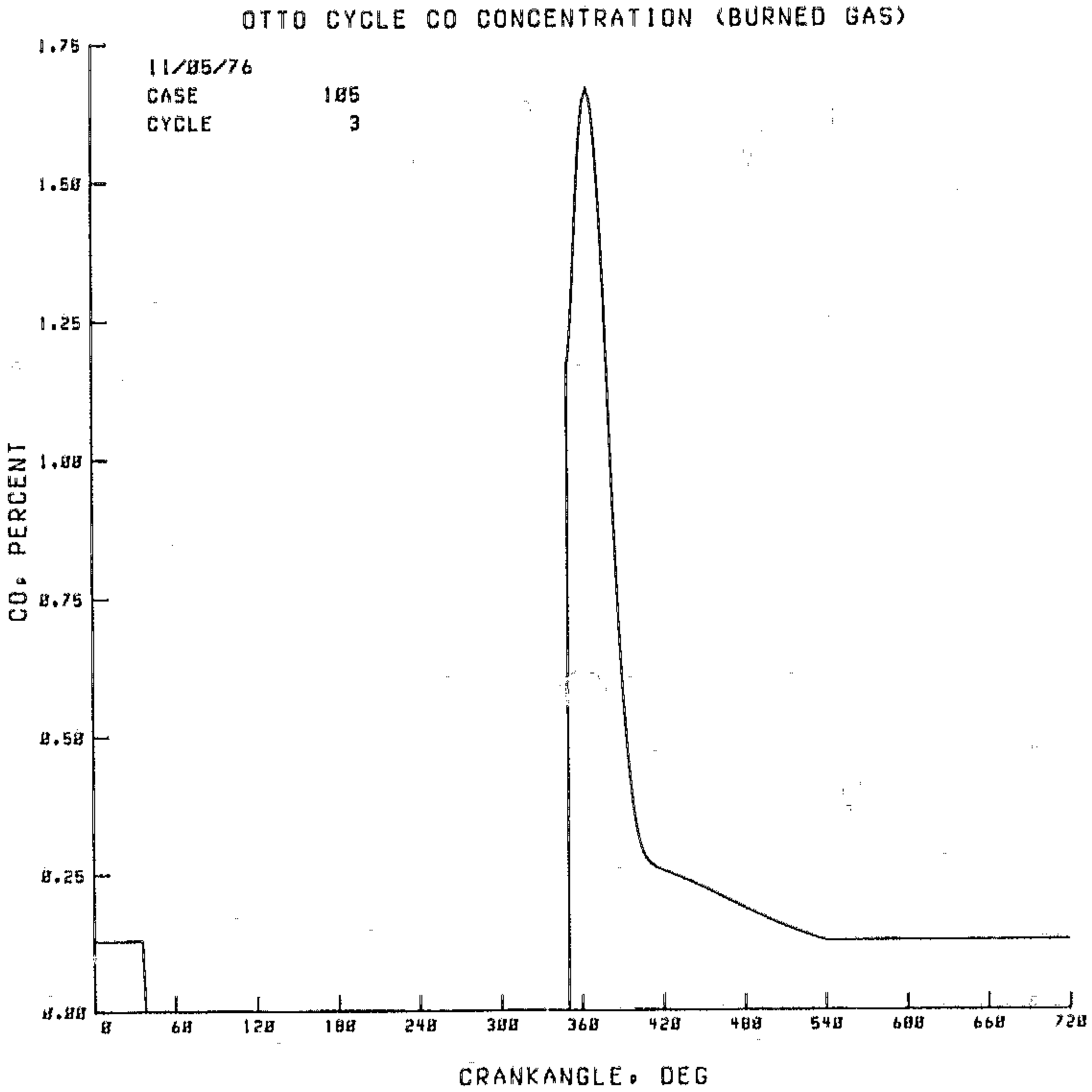

Fig. 5 - Calculated burned gas carbon monoxide concentration for equilibrium chemistry

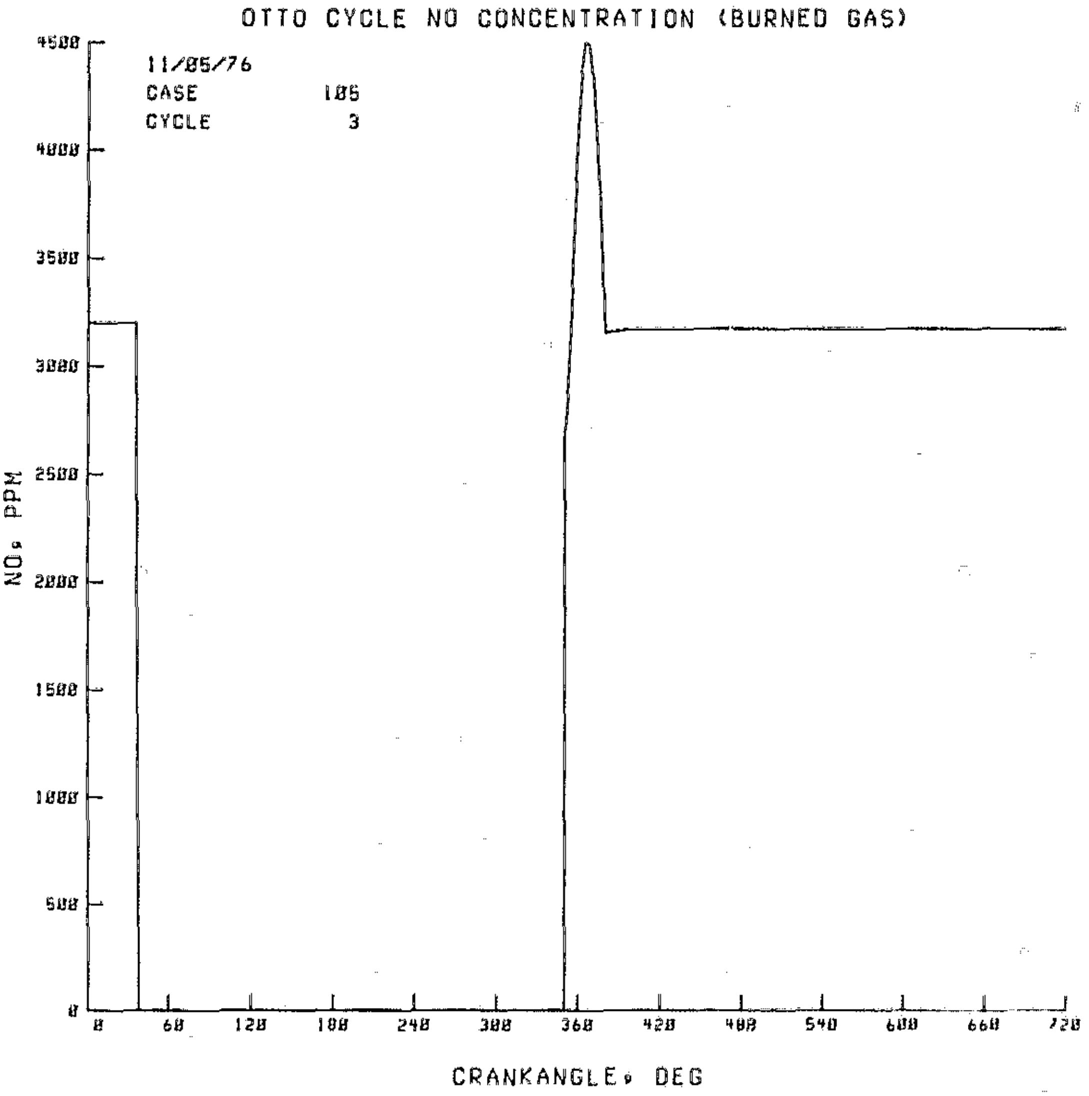

Fig. 6 - Calculated burned gas nitric oxide concentration for equilibrium chemistry

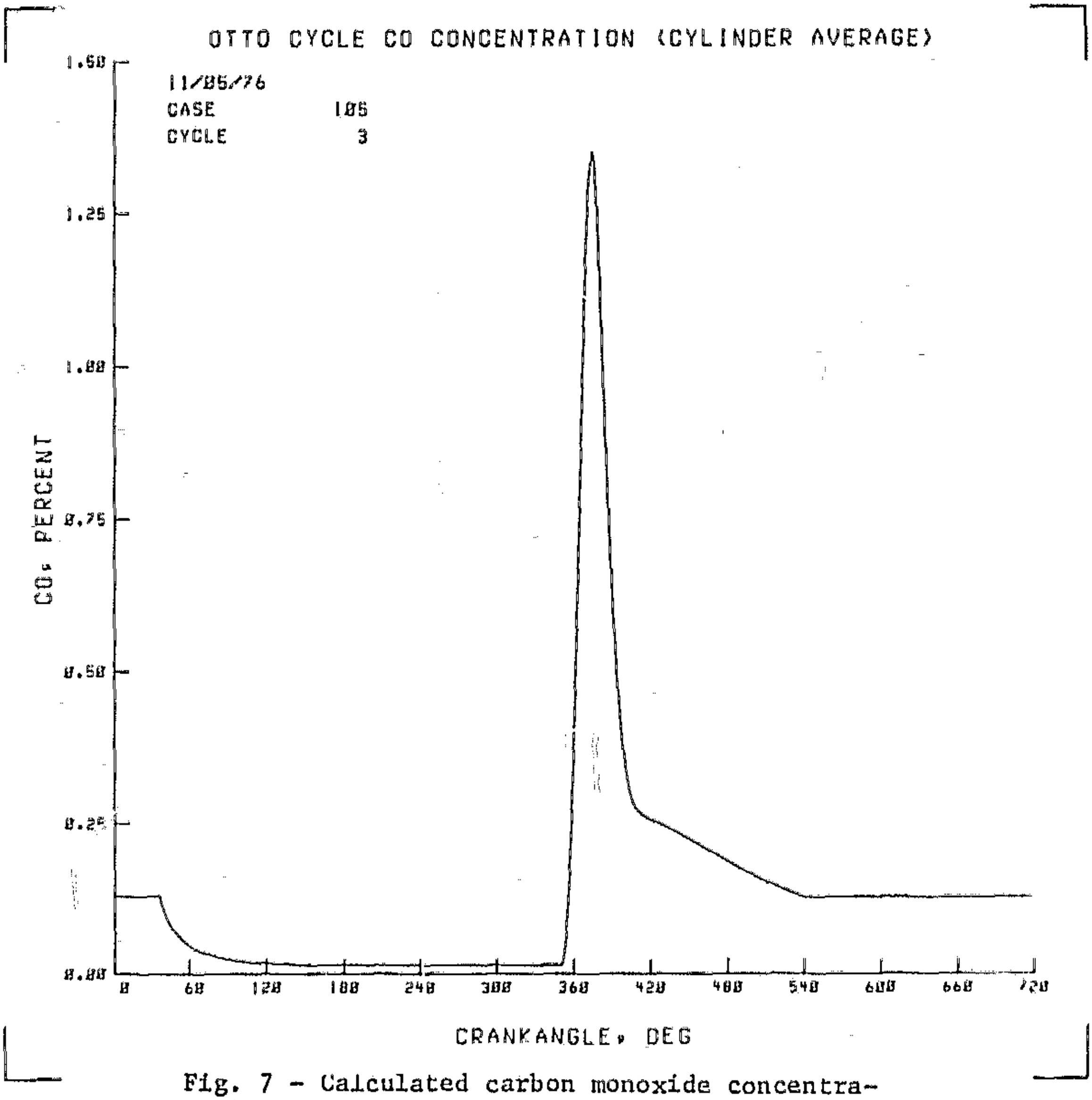

Fig. 7 - Calculated carbon monoxide concentration in the cylinder for equilibrium chemistry

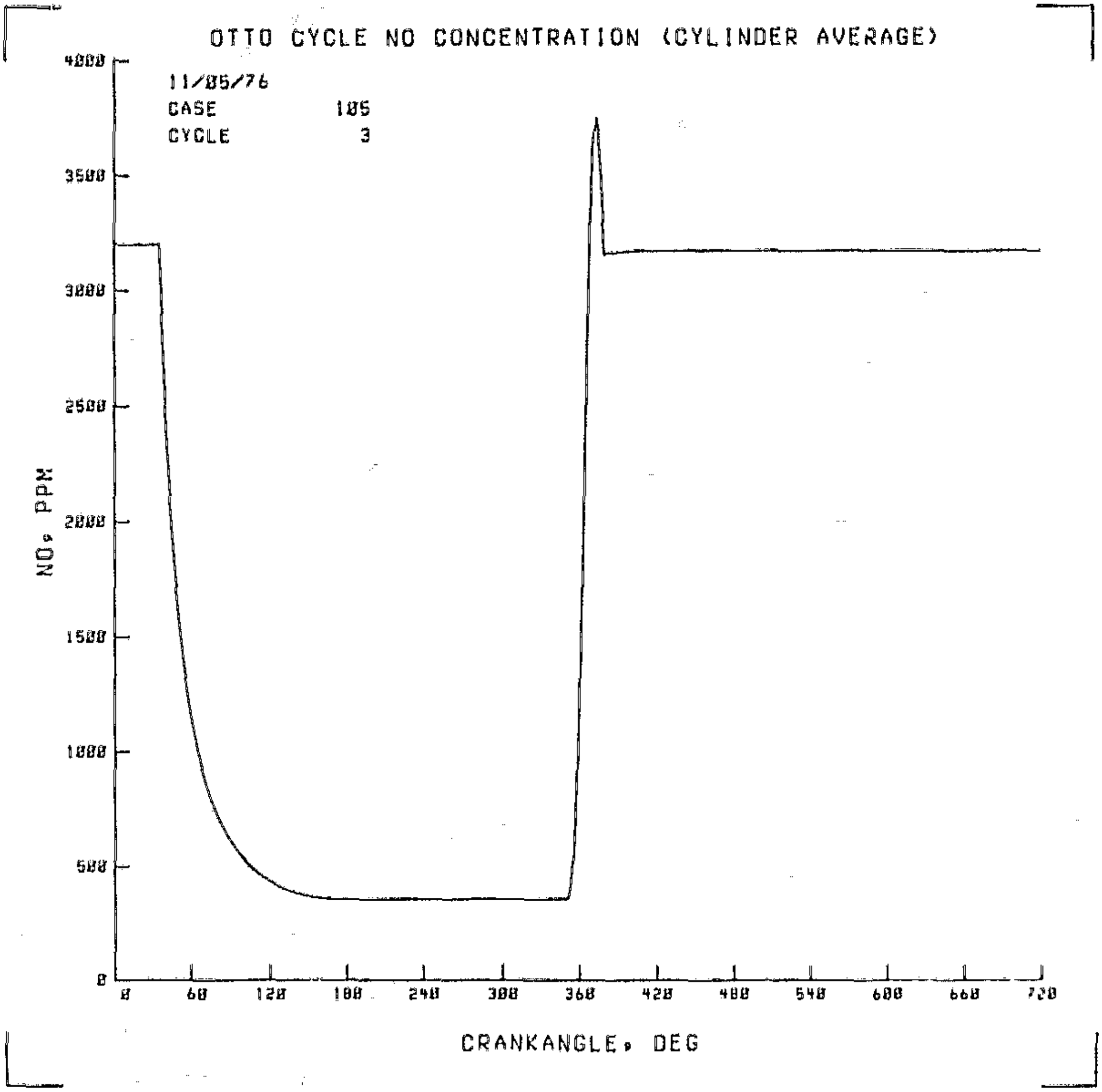

Fig. 8 - Calculated nitric oxide concentration in the cylinder for equilibrium chemistry

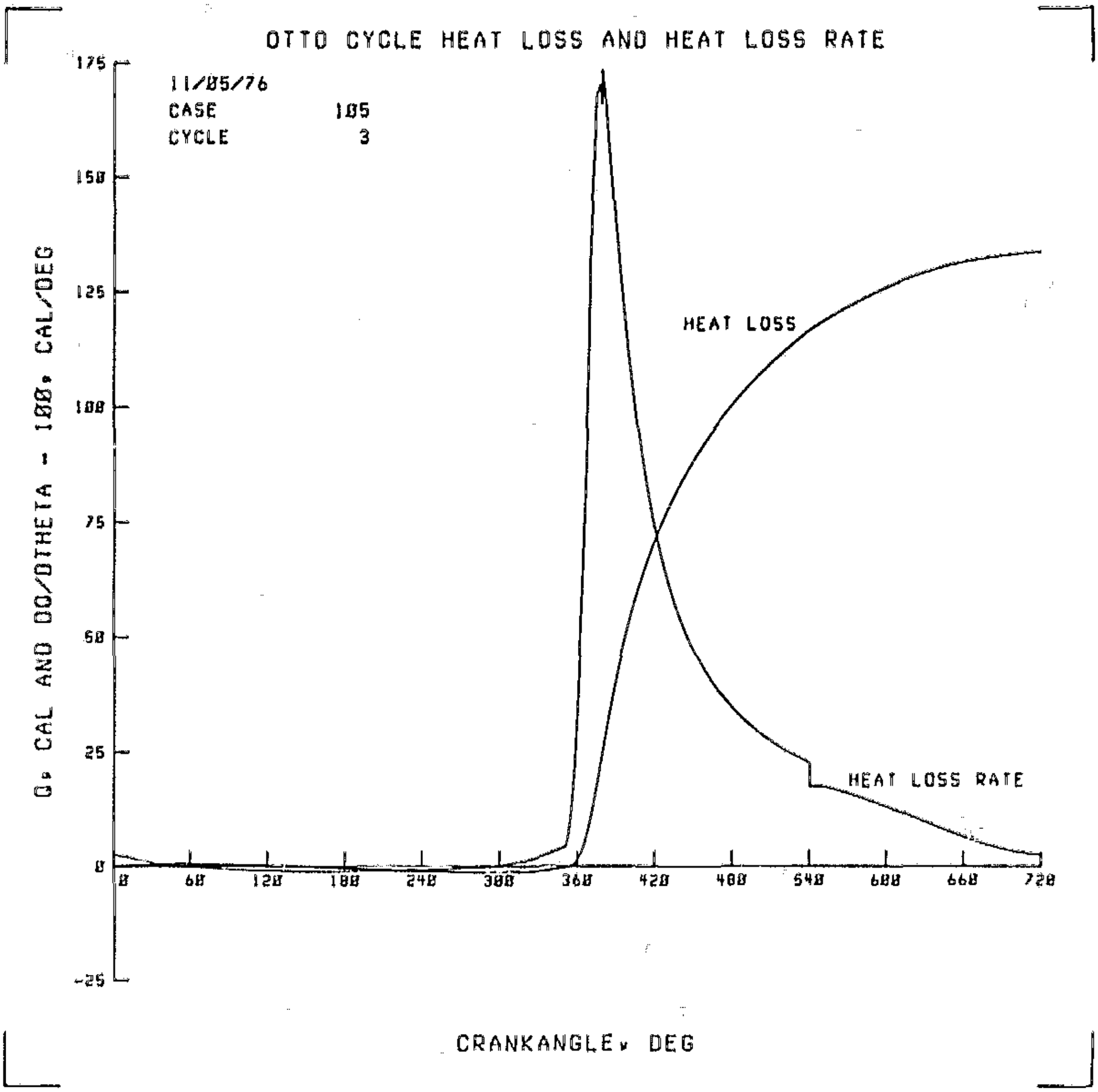

Fig. 9 - Calculated heat loss and heat loss rate for the Eichelberg heat transfer correlation

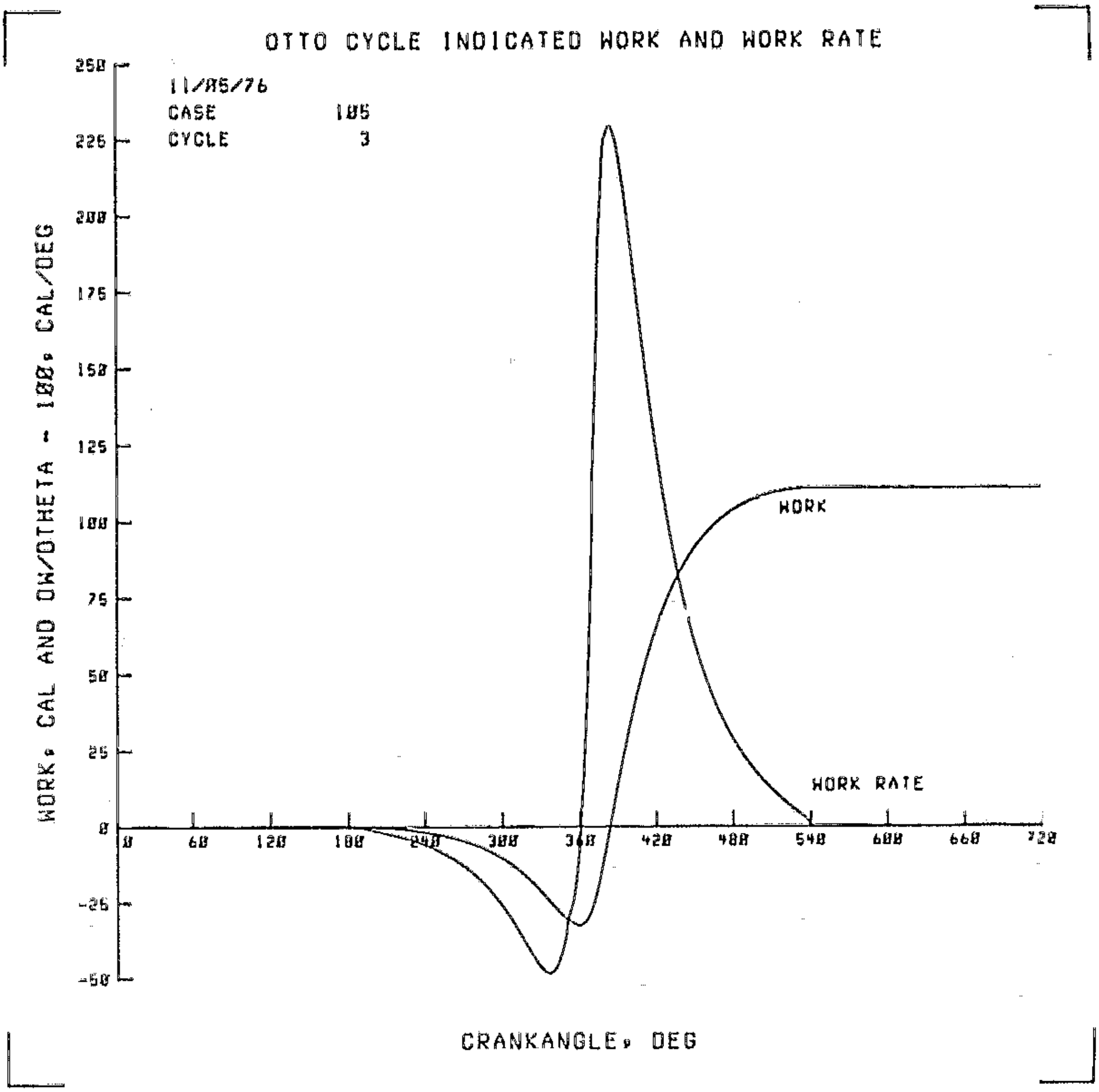

Fig. 10 - Calculated work and work rate

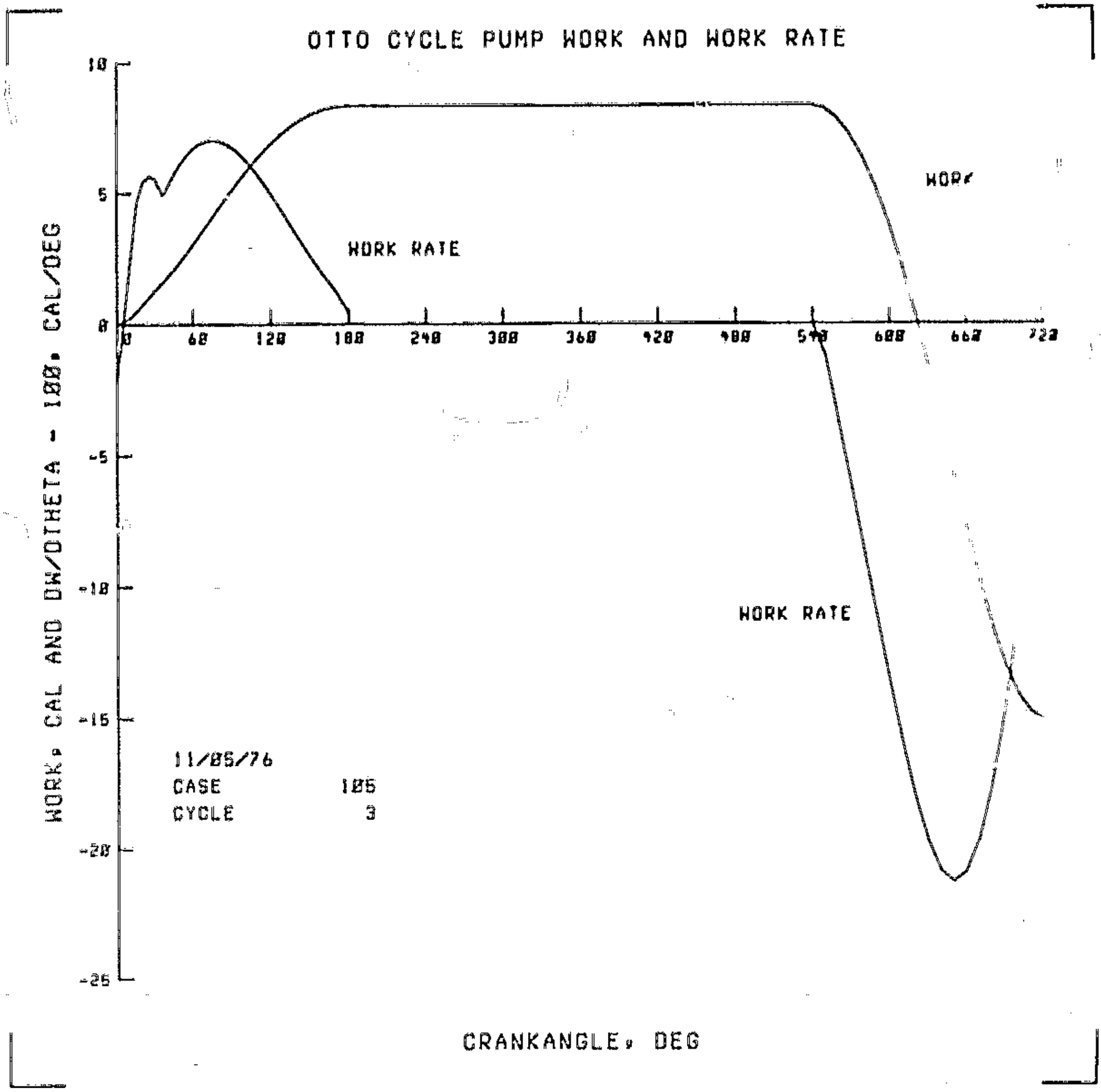

Fig. 11 - Calculated pump work and pump work rate

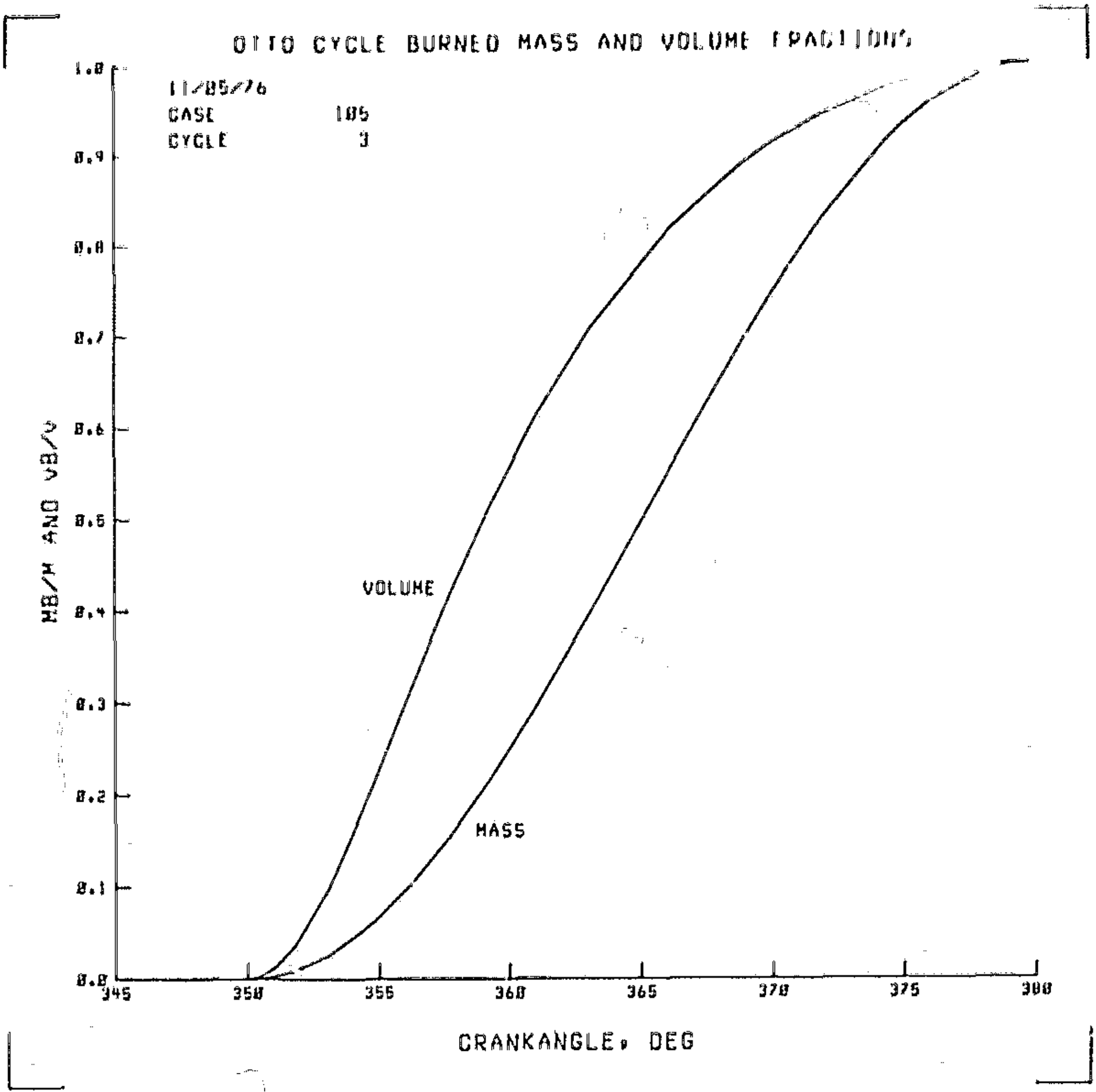

Fig. 12 - Calculated burned mass and volume fractions

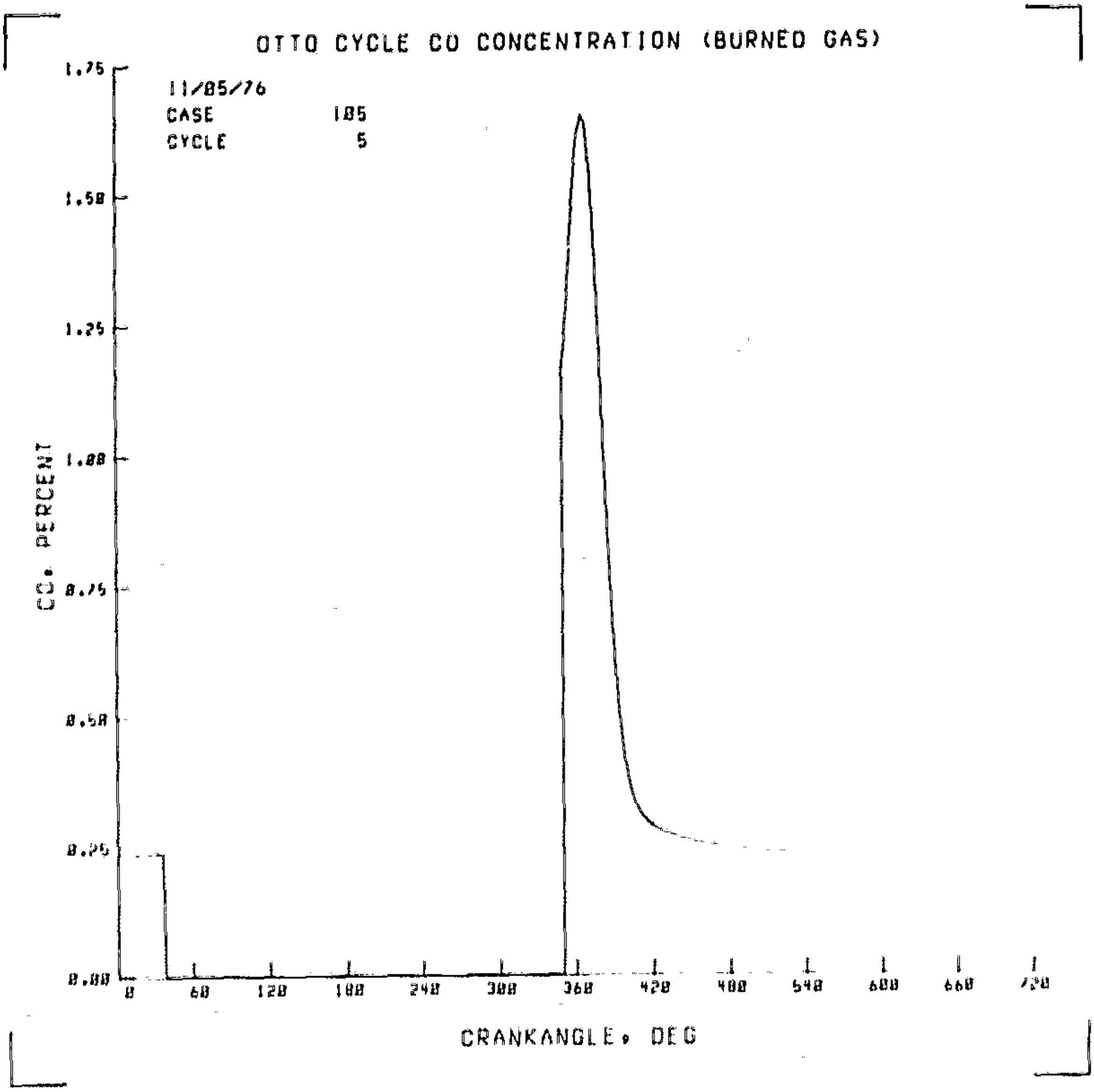

Fig. 13 - Calculated burned gas carbon monoxide concentration for finite rate chemistry

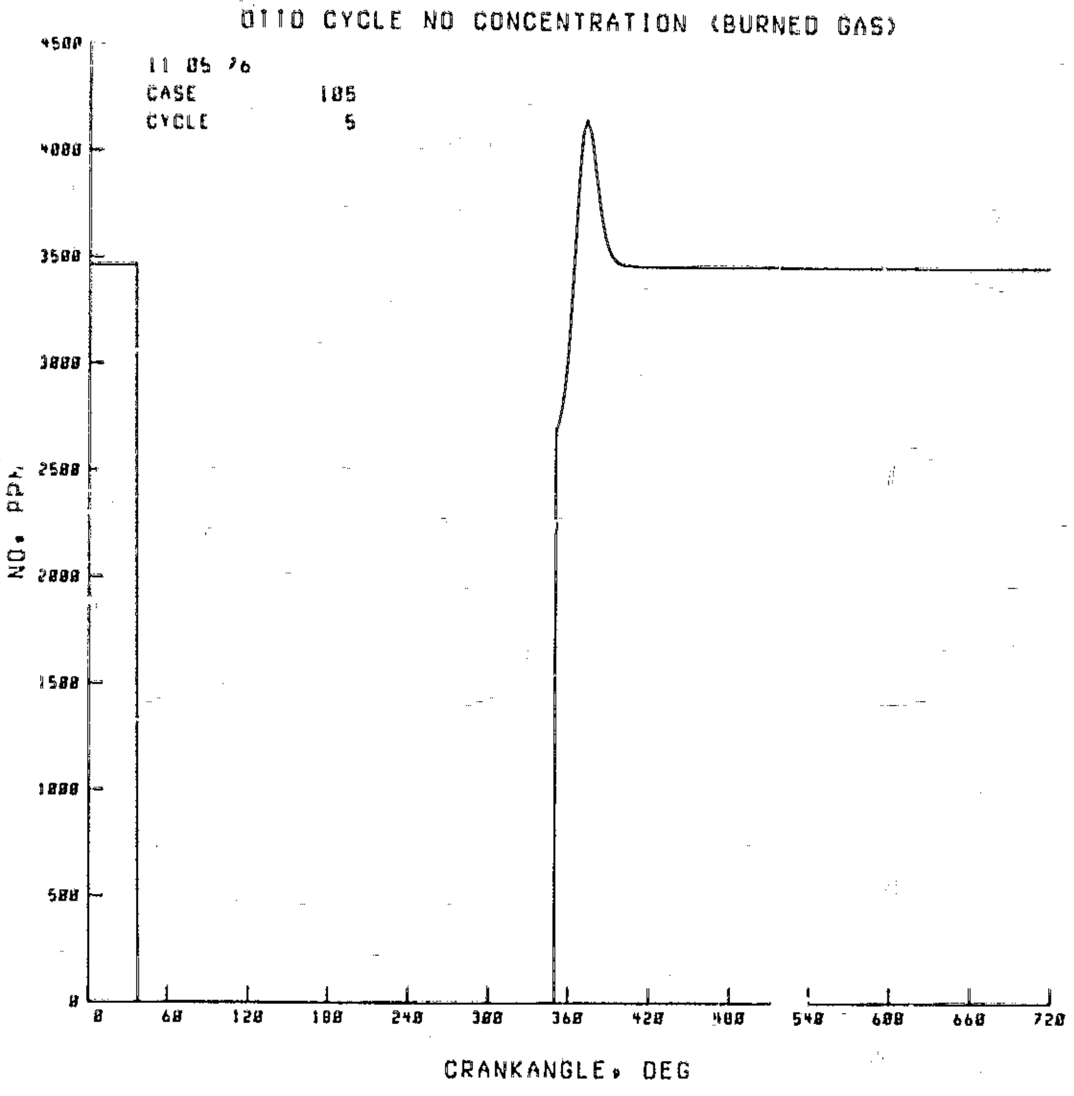

Fig. 14 - Calculated burned gas nitric oxide concentration for finite rate chemistry

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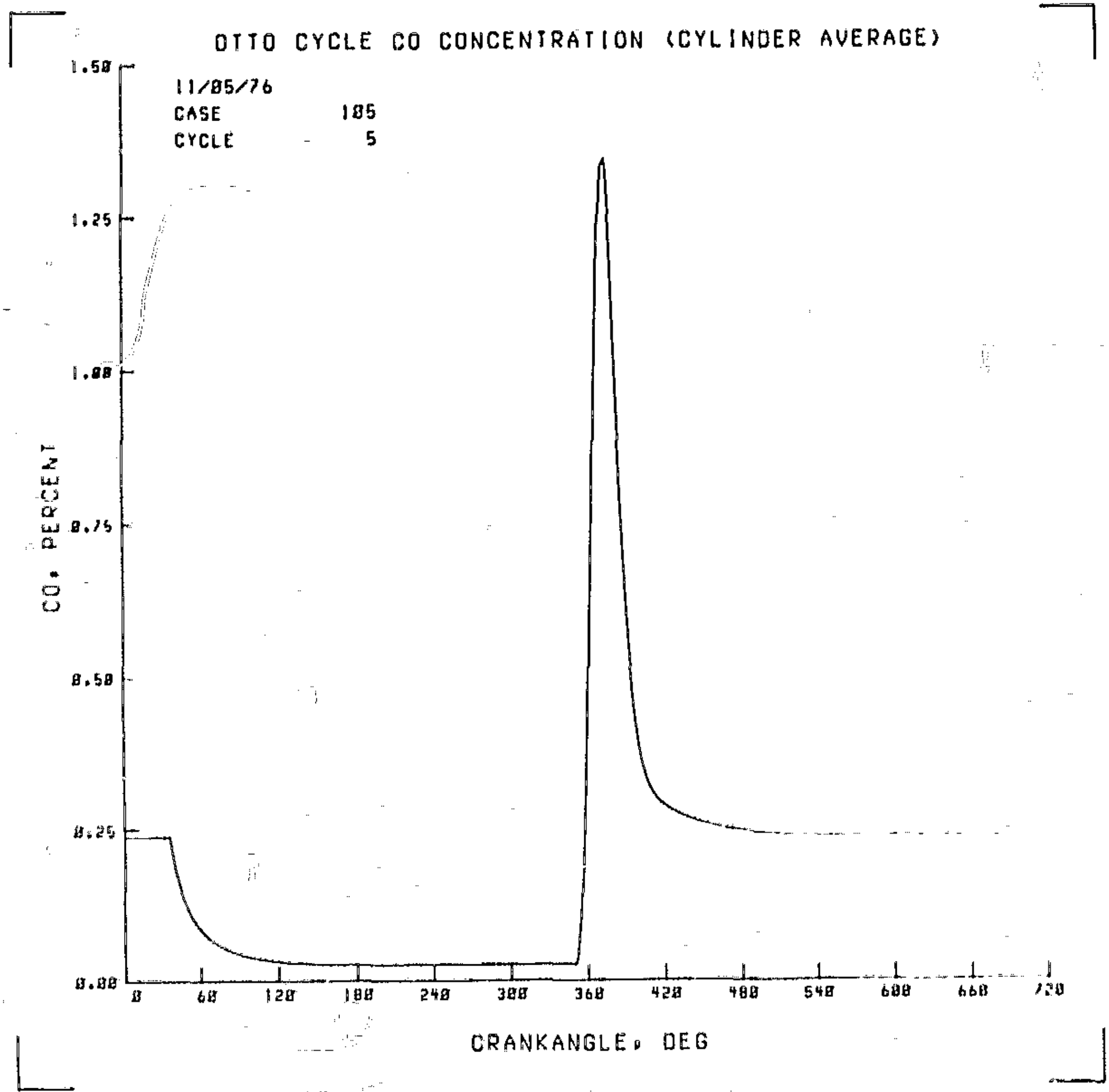

Fig. 15 - Calculated carbon monoxide concentration in the cylinder for finite rate chemistry

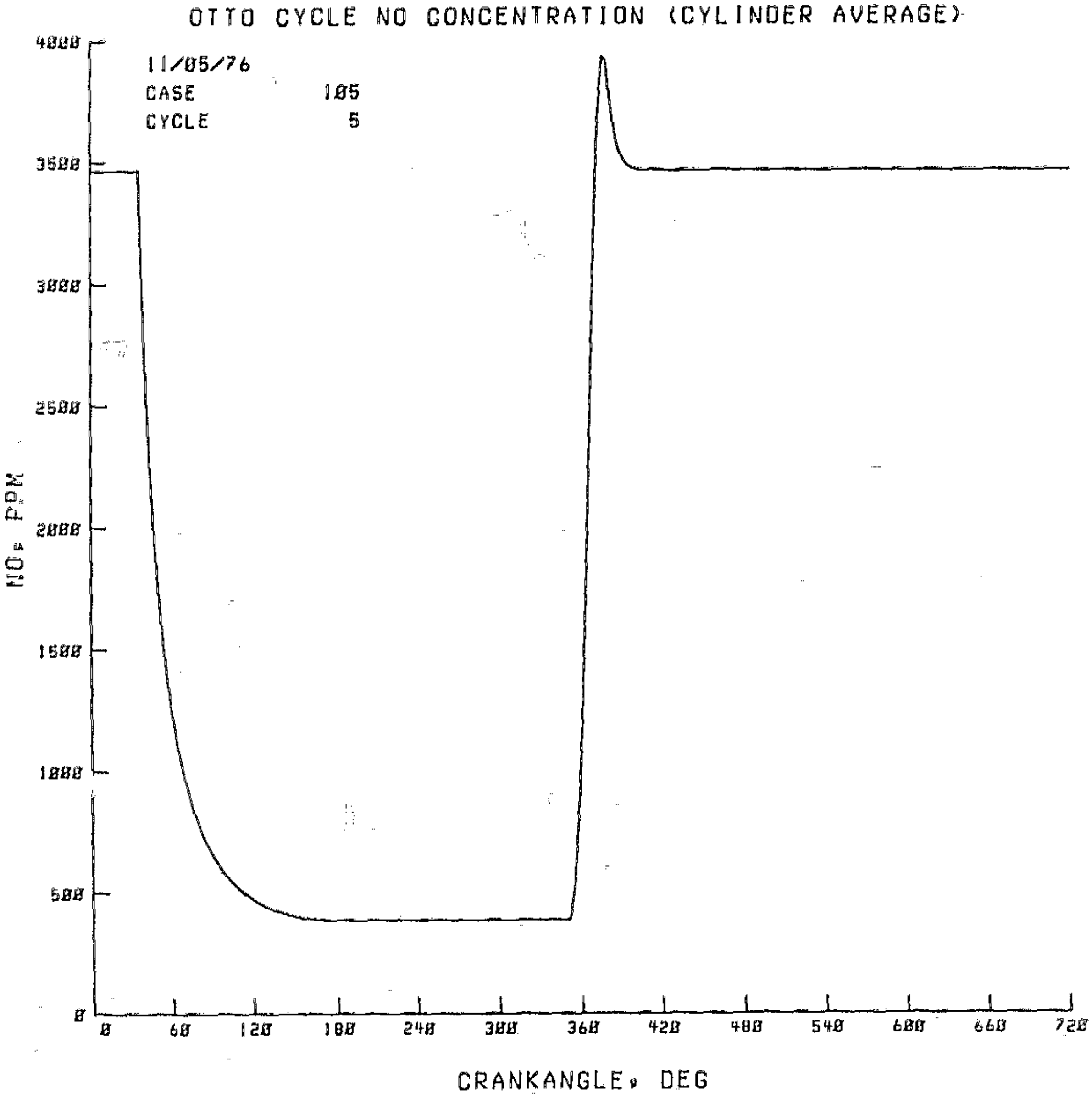

Fig. 16 - Calculated nitric oxide concentration in the cylinder for finite rate chemistry

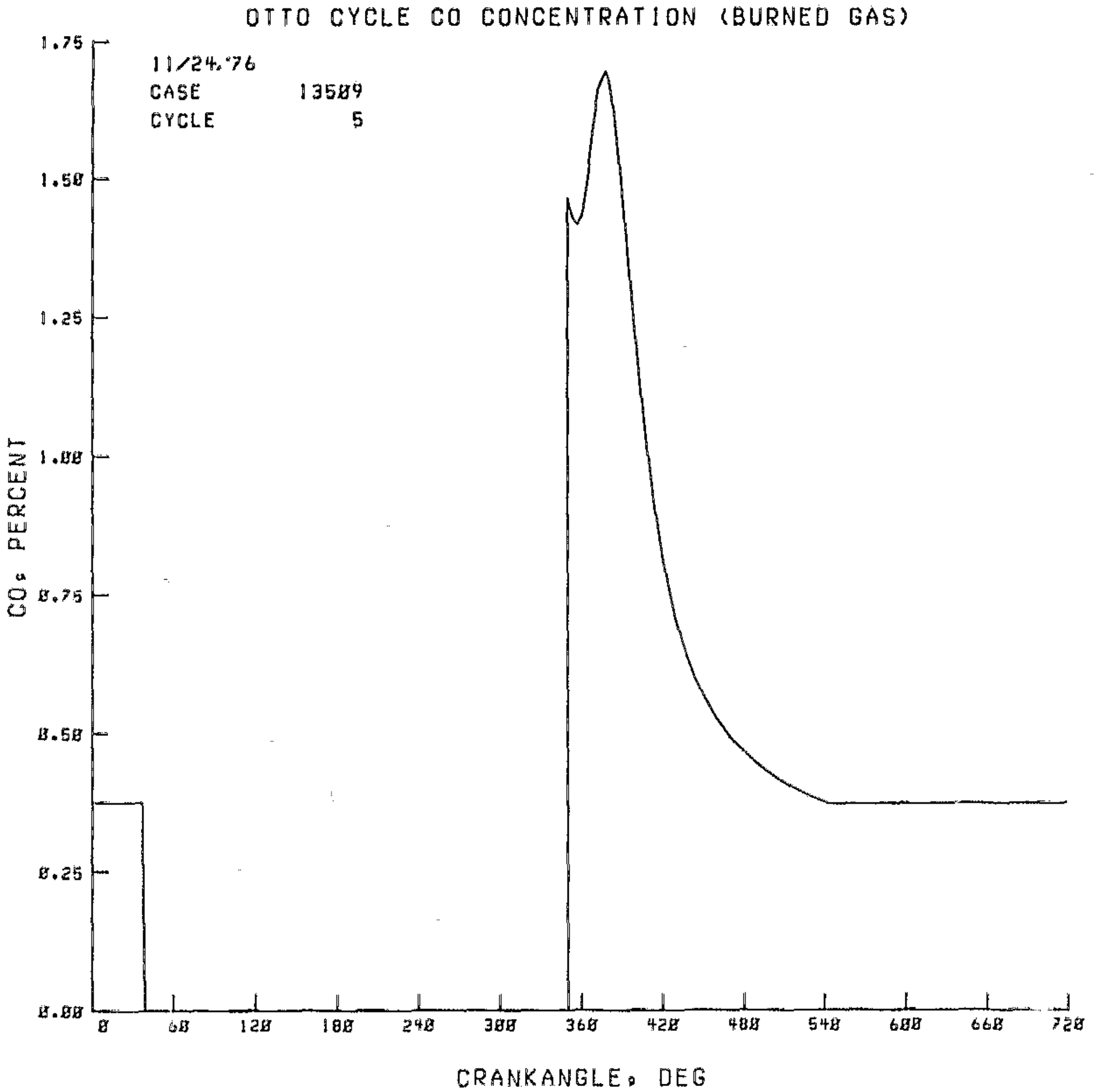

Fig. 17 - Calculated carbon monoxide concentration in the burned gas for $\tau = 0.0009$ and finite rate chemistry

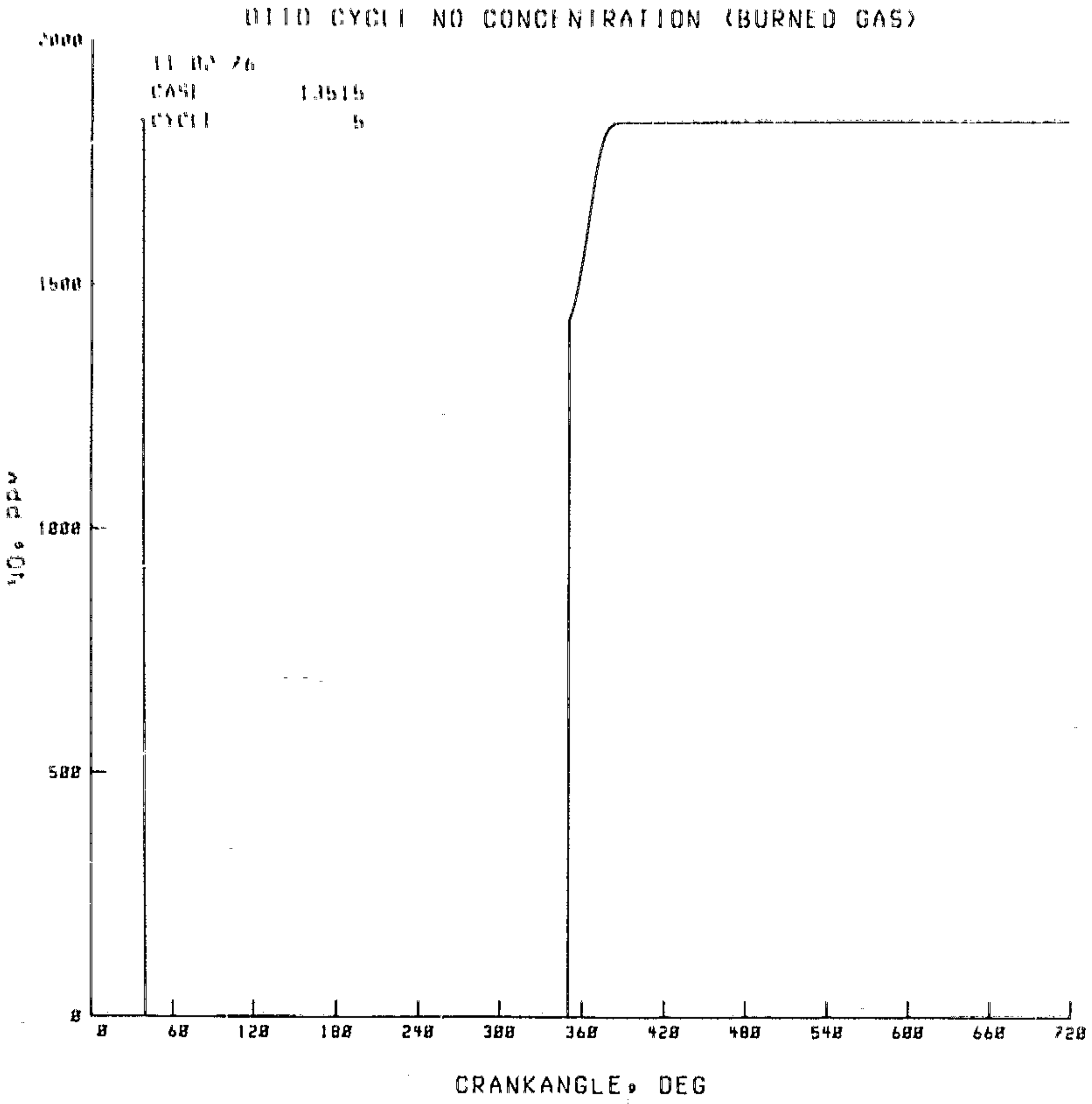

Fig. 18 - Calculated nitric oxide concentration in the burned gas for 15% exhaust gas recirculation and finite rate chemistry