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THEORETICAL STUDY OF REACTIVE FLUID FLOW IN HETEROGENEOUS COMBUSTION PROCESSES

Final Report
NASA Grant No. NGR 47-005-085
National Aeronautics and Space Administration
Washington, D. C. 20546

Submitted by:

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Research Laboratories for the Engineering Sciences

University of Virginia

Charlottesville

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ABSTRACT

A computational method has been developed to study the transient phenomena of reactive fluid flows in a hybrid rocket system consisting of solid fuel and liquid oxidizer undergoing heterogeneous combustion. In this system, the liquid oxidizer is injected into the center cavity of the solid fuel, it subsequently vaporizes and flows axially through the fuel cavity. Initial ignition provides the heat necessary to vaporize the solid fuel which mixes with the gaseous oxidizer and ignites to sustain the continuous combustion.

The species, momentum and energy conservation equations for the gas phase have been derived for a transient, two-dimensional, turbulent flow of an N-component gas mixture with chemical reactions. The governing equation in the solid phase is the transient, two-dimensional, heat conduction equation with no heat source or sink. Heat and mass transfer coupling between the solid and the gas phases is assumed in the derivation of boundary equations at the interface. A cylindrical co-ordinate system is used throughout the derivation of all governing equations.

The appropriate finite-difference schemes of second order accuracy have been selected for the numerical solution of these highly-coupled, second-order, non-linear, partial differential equations. An implicit Lax-Wendroff scheme for the gas phase equations, an implicit Crank-Nicolson scheme for the transient heat conduction equation, and, a time-independent finite-difference scheme for the boundary equations have been employed in deriving the difference equations for computer programming.

In order to gain insight into the numerical problem involved, additional assumptions have been made as follows: (a) constant fluid properties; (b) constant turbulent values for viscosity, thermal conductivity and diffusion coefficient; (c) a one-step overall irreversible reaction, e.g., fuel + oxidizer → product; and (d) constant rate of mass addition from fuel surface.

For a simple case with aluminum as the fuel, oxygen as the oxidizer and aluminum oxide as the product, numerical calculations have been performed with the following necessary initial, boundary and physical conditions:

(a) Flow of the gaseous oxidizer is accelerated to a given initial velocity with mass addition from the solid fuel surface.

(b) The initial temperature profile corresponds to the conditions when ignition has just been completed.

(c) Inlet conditions and temperature at the exterior surface of the solid fuel are constant.

(d) The axial component of velocity is assumed to be zero at the interface and the radial component of velocity is required to be zero at the center line.

(e) A favorable downstream pressure gradient is imposed.

(f) The Reynolds number has a value corresponding to the region for turbulent flow.

The transient solutions obtained indicate a smooth transition from initial to steady-state conditions which allows a study of the transient phenomena in heterogeneous combustion processes. At any axial position,

the temperature corresponding to the reaction zone initially increases, and, as the relatively cold oxygen supply from the inlet arrives, the temperature decreases until the steady-state condition is reached. As expected, where there is chemical reaction, aluminum oxide is produced, and, aluminum and oxygen are depleted. The temperature changes in the reaction zone have a strong influence on the rate of production of aluminum oxide.

The steady-state results indicate a sharp temperature peak near the fuel surface and a decrease in the magnitude of the axial velocity gradient at the fuel surface which are in good qualitative agreement with available experimental steady-state data.

ACKNOWLEDGEMENTS

This research has been conducted under NASA Grant No. NGR-47-005-085. Dr. A. R. Saunders initiated and monitored this research project through NASA, Langley Research Center.

Drs. K. R. Hall and J. L. Gainer have made contribution to the numerical schemes and the transport properties, respectively. Drs. B. A. Chartres and R. S. Stepleman have been consulted on various subjects concerning numerical analysis.

Initial computation was carried out at the Computing Center, University of Virginia, through a grant from the University of Virginia. The major computation was performed through the use of the CDC6600 computers at NASA, Langley Research Center.

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LIST OF SYMBOLS

Å	Angstrom
Btu	British thermal unit
C_p	Specific heat per unit mass of gas mixture at constant pressure
$\hat{C}_p$	$\frac{C_p}{C_{po}}$
C_s	Specific heat per unit mass of solid fuel
$\hat{C}_s$	$\frac{C_s}{C_{so}}$
D_i	Binary diffusion coefficient of the ith chemical species into the rest
$\hat{D}_i$	$\frac{D_i}{D_o}$
E	Activation energy
Ec	Eckert number, $\frac{v_o^2}{C_{po}\ T_o}$
ft	Feet
g	Gas
g-mole	Gram-mole
h	Enthalpy per unit mass of gas mixture
$\hat{h}$	$\frac{h}{C_{po}\ T_o}$
h_i°	Heat of formation per unit mass of the ith chemical species
h_{Li}	Latent heat per unit mass of the ith chemical species due to phase change

LIST OF SYMBOLS (continued)

$h_{\ell g}$	Heat of vaporization per unit mass
h_{sg}	Heat of sublimation per unit mass
$h_{s\ell}$	Heat of fusion per unit mass
hr	Hour
in	Inch
k	Specific reaction rate coefficient (rate constant)
kcal	Kilocalorie
ℓ	Liquid
L	Length of combustion chamber
M	Molecular weight
N	Number of chemical species present in the combustion chamber
psf	Pound force per square foot
P	Static pressure of gas mixture
$\hat{P}$	$\frac{P}{\rho_o v_o^2}$
Pr	Prandtl number, $\frac{C_{po} \mu_o}{\lambda_o}$
r	Radial distance
r_e	External radius of combustion chamber
r_o	Internal radius of combustion chamber
$\hat{r}$	$\frac{r}{r_o}$
$\dot{r}$	Regression rate of fuel surface
$\hat{\dot{r}}$	$\frac{\dot{r}}{\dot{r}_o}$
R	Gas constant or Rankine temperature scale

LIST OF SYMBOLS (continued)

$\hat{R}_i$	$\frac{R_i}{C_{po}}$
Re	Reynolds number, $\frac{r_o \rho_o v_o}{\mu_o}$
S	Steric factor
Sc	Schmidt number, $\frac{\mu_o}{\rho_o D_o}$
sec	Second
t	Time
$\hat{t}$	$\frac{t v_o}{r_o}$
T	Temperature of gas mixture
$\hat{T}$	$\frac{T}{T_o}$
T_s	Temperature of solid fuel
$\hat{T}_s$	$\frac{T_s}{T_{so}}$
u	Any one of the dependent variables in dimensionless form
v_r	Radial velocity component
$\hat{v}_r$	$\frac{v_r}{v_o}$
v_z	Axial velocity component
$\hat{v}_z$	$\frac{v_z}{v_o}$
W_i	Rate of production of the ith chemical species per unit volume

LIST OF SYMBOLS (continued)

$\hat{W}_i$	$\frac{W_i}{W_o}$
y_i	Mass fraction of the ith chemical species
z	Axial distance
$\hat{z}$	$\frac{z}{r_o}$
α_o	Characteristic thermal diffusivity of gas mixture, $\frac{\lambda_o}{\rho_o C_{po}}$
α_{so}	Characteristic thermal diffusivity of solid fuel, $\frac{\lambda_{so}}{\rho_{so} C_{so}}$
γ	$\frac{L}{r_o}$
β	$\frac{r_e}{r_o}$
Δr	Radial grid size
$\Delta\hat{r}$	$\frac{\Delta r}{r_o}$
Δt	Time increment
$\Delta\hat{t}$	$\frac{\Delta t v_o}{r_o}$
Δz	Axial grid size
$\Delta\hat{z}$	$\frac{\Delta z}{r_o}$
ζ	Maximum tolerance allowed
η	Maximum relative error allowed
λ	Thermal conductivity

LIST OF SYMBOLS (continued)

$\hat{\lambda}$	$\frac{\lambda}{\lambda_o}$
$\hat{\lambda}_s$	$\frac{\lambda_s}{\lambda_{so}}$
μ	Viscosity of gas mixture
$\hat{\mu}$	$\frac{\mu}{\mu_o}$
μ_B	Bulk viscosity of gas mixture
ν_i'	Stoichiometric coefficient of the ith reactant
ν_i''	Stoichiometric coefficient of the ith product
π	3.14159..
ρ	Density of gas mixture
$\hat{\rho}$	$\frac{\rho}{\rho_o}$
$\hat{\rho}_s$	$\frac{\rho_s}{\rho_{so}}$
σ_{12}	Average diameter of colliding species

Subscripts

i	The ith chemical species in the gas mixture
j	Index for iteration
m	Index for radial grid points
n	Index for axial grid points
s	Corresponding value for solid fuel
w	Corresponding value at the gas-solid interface
o	Characteristic value

CHAPTER I

INTRODUCTION

Although the concept of heterogeneous combustion has been the concern of industrial and fire research for some time, it has only recently become a subject of general interest in the aerospace industry. Recent recognition of the potential advantage of hybrid rocket systems over the conventional solid-propellant or liquid-propellant rocket systems, the problem of ablation during re-entry of space vehicle, etc., call for for more research efforts, both theoretically and experimentally, in the area of heterogeneous combustion. This work is concerned mainly with the theoretical aspect of heterogeneous combustion as applied to hybrid rocket systems.

An idealized hybrid rocket system can be sketched schematically as shown in Figure I.I. The liquid oxidizer is injected into the center cavity of the solid fuel. It is assumed to be completely vaporized and flows axially through the center core of the solid fuel. After ignition, the gas phase combustion of the fuel and oxidizer provides the heat necessary to vaporize more fuel and sustain the continuous combustion.

The actual reaction taking place inside the rocket system is quite complex. This situation is characterized by transient behavior, variable fluid and transport properties, simultaneous heat and mass transfer, coupled radiative and convective effects, a receding fuel surface, complicated chemical kinetics and turbulence.

In the interior-ballistic design of such a rocket system, it is pertinent to require a prediction of the rate of fuel consumption as a

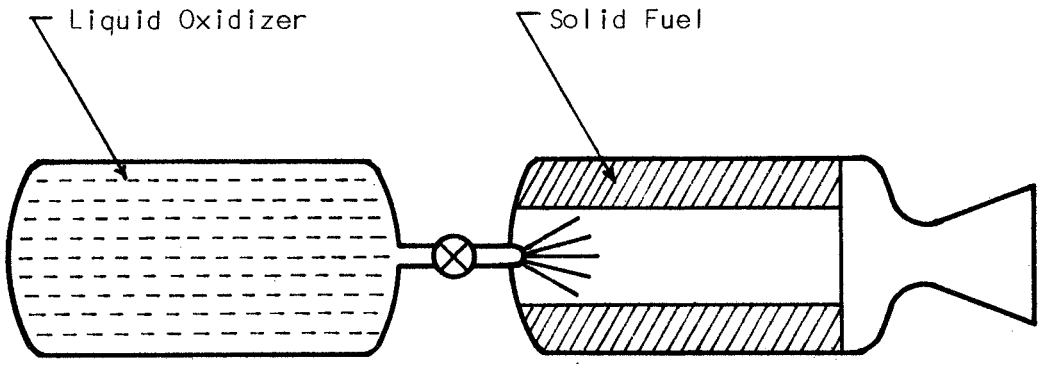


Figure 1.1 "Idealized" Hybrid Rocket System

function of axial position and the rate of oxidizer injection. Hence, early analytical effort was centered primarily on the development of regression rate equations which were expressed in terms of known thermodynamic or thermochemical parameters. A survey of published literature indicates that previous analyses of hybrid rocket systems are limited to the "chemical equilibrium" flow in a steady, laminar or turbulent boundary layer with heat and mass transfer, and, constant fluid and transport properties. It is apparent that there is a lack of understanding of the non-equilibrium aspect of the problem.

The current analysis adopts an overall approach with a view to gaining a basic understanding of the fundamental processes involved in hybrid rocket systems. Mathematical formulation of the governing equations to describe the physical system has been carried out in the most general fashion possible. Numerical solution of these governing equations is sought. Mathematical modeling of the physical mechanisms involved has been performed for a simple case. More sophisticated mathematical models will be incorporated one at a time until eventually a computational method is developed which simulates realistic experimental conditions.

The development of high speed digital computers has made it possible to attempt a numerical solution of a number of physical problems that have no closed-form analytical solutions. Over the years, a number of numerical schemes of higher accuracy have been developed to cope with the demand. Numerical solutions of a wide variety of previously unsolved problems in the field of engineering and the sciences have been reported. However,

currently, the maximum storage available in any of the existing computers is still insufficient to handle any transient, three-dimensional problem. Also, the computational time required for a numerical solution must be kept within reasonable limit from the economic view point.

With these limitations in mind, the mathematical formulation is carried out within the framework of a transient, two-dimensional problem. The main simplifying assumptions are as follows: (a) turbulent flow of oxidizer over fuel with negligible turbulence intensity; (b) negligible radiative effects; and (c) non-receding fuel surface. The cylindrical coordinate system is used throughout for the derivation of all governing equations.

The species continuity, momentum, and energy equations for the gas phase have been derived for a transient, two-dimensional, turbulent flow of an N-component gas mixture with chemical reactions. The governing equation in the solid phase is the transient, two-dimensional, heat conduction equation with no heat source or sink. Heat and mass transfer coupling between the solid and gas phase is assumed in the derivation of boundary equations at the interface.

The appropriate finite-difference schemes of second-order accuracy have been selected for the numerical solution of these highly-coupled, second-order, non-linear, partial differential equations. An implicit Lax-Wendroff scheme for the gas phase equations, an implicit Crank-Nicolson scheme for the transient heat conduction equation, and a time-independent finite-difference scheme for the boundary equations have been employed in deriving the difference equations for computer programming.

Numerical checkout of these difference equations has been performed. Since these difference equations are highly-coupled, the incorporation of both a conservative relaxation procedure and an accelerating convergence procedure (Aitken's δ^2-method) has been found necessary. Significant reduction of roundoff errors has been achieved and the proper convergence criteria have been established.

In order to carry out a numerical solution of these difference equations, additional methematical models have been formulated to describe the physical mechanisms involved. The assumptions made are as follows: (a) constant fluid and transport properties by using equivalent turbulent values for viscosity, conductivity and diffusion coefficient; (b) one-step overall irreversible chemical reaction, e.g., oxidizer + fuel → products; (c) constant rate of mass addition from the fuel surface. In addition, the physical parameters and the property values are chosen such that the Reynolds number has a value corresponding to the region for turbulent flow. With the necessary initial and boundary conditions, numerical calculations have been performed for a simple case with aluminum as the fuel, oxygen as the oxidizer and aluminum oxide as the product.

The critical time increment has been determined empirically to be in the range of 3 - 6 microseconds. The first computed results indicated that the initially ignited flame had been blown out by the relatively cold oxygen from the inlet. With modified values for the reaction orders, the newly computed results show that a sustaining flame is indeed possible. The sustaining flame is in a region very close to the fuel surface. Also, mass addition and combustion cause a decrease in the magnitude of the

axial velocity gradient at the fuel surface. These phenomena are in good qualitative agreement with available steady-state experimental data. With more sophisticated models to describe the physical mechanisms involved, it is believed that such a computational method can be used to simulate realistic experimental conditions.

CHAPTER II

SURVEY OF PREVIOUS ANALYSIS

A search for published literature on the heterogeneous combustion of hybrid rocket systems has been conducted. The models used in the previous analysis are classified and presented here. Previous analyses which are considered to be characteristics of hybrid rocket systems are discussed.

A. Previous Analytical Models

The analytical models used by previous workers in their analysis of hybrid rocket systems can be classified into the following three categories: tube combustion model, film combustion model and turbulent boundary layer model. A description of these models is felt necessary to allow the reader to get acquainted with the problem and to appreciate the current analytical effort.

1. Tube Combustion Model

Bartel and Rannie (1) considered a model for a slow-burning fuel. In their model sketched in Figure II.1, the solid fuel is in the form of a tube through which passes a one-dimensional, turbulent flow of air entering at bulk velocity, v_o, density, ρ_o, and total temperature, T_{to}. The diffusion of oxygen through the gas film to the fuel surface was assumed to be the rate-controlling factor. Stoichiometric reaction was assumed but no assumption as to the location or structure of the flame was made. Instead, it was assumed that the ratio of oxygen in the gas

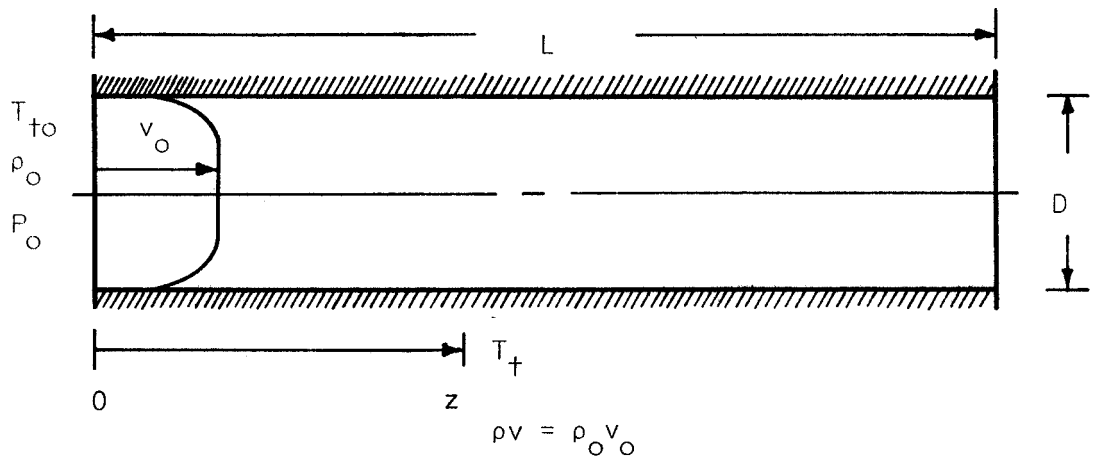


Figure II.1 Tube Combustion Model of Bartel & Rannie

at any axial position, z, to the entering oxygen concentration is a function of the total temperature at that axial position. Using the conventional pipe-flow expression for the friction coefficient, Bartel and Rannie obtained an expression for the total burning rate of fuel. It was reported that this expression correlated well with experimental data on carbon fuel.

Penner (2) also considered a model in the form of a hollow cylinder of fuel burning internally as oxygen flows through it. Again, a diffusion-controlled burning rate was assumed. Using the Burke-Schumann approximation for laminar flow, Penner derived a closed-form solution for the oxygen distribution as a function of radial and axial position in the core region of the tube. The flame was assumed to be infinitesimal in thickness and arbitrarily located at the edge of the laminar boundary layer. The mass burning rate of fuel was computed by assuming no fuel flow in the axial direction. A fit of Penner's solution to experimental data on the combustion of Plexiglass tubes in oxygen was reported by Peck (3).

Fineman (4) considered both laminar and turbulent flows in a tube using Spalding's expression for mass transfer in the "stagnant film" approximation (5). The "film" thickness was arbitrarily identified with the thickness of the boundary layer in the tube entrance for the turbulence case. Mass transfer effects upon the boundary layer thickness and upon flow in the core were neglected. It was reported that the calculated results compared reasonably well with the experimental data of Peck and Lodwig (6) on Plexiglass burning in oxygen.

Using the Chilton-Colburn modification of the Reynolds analogy between mass and momentum transfer, Green (7) showed that the result

derived by Bartel and Rannie (1) can be generalized by using Spalding's mass transfer number to predict average fuel burning rate for a slow-burning system without any adjustment of empirical constants. The derived expression agreed with experimental data reported by Houser (8) and is recommended for use in preliminary design of hybrid rocket systems.

Smoot and Price (9) extended the Colburn analogy approach to derive a regression rate equation including the effects of condensed species at the wall. Numerical evaluations of six thermodynamic and transport parameters are required to predict the local regression rate. Theory was compared with experimental data on regression rates for non-metalized and metalized hybrid fuel systems (10, 11). Good agreement was reported for low oxidizer flow rate, but, the model could not account for the observed pressure dependence at high oxidizer flow rates.

2. Film Combustion Model

Analyses of the combustion of liquid fuel have been developed by Spalding (5, 12) and was first adapted by Emmons (13) to the fuel drop problem. Mortet and Barrere (14) employed Emmon's model for the hybrid problem. The film combustion model of Emmons is sketched as shown in Figure 11.2. Finite rate reaction of fuel and oxidizer was assumed in a laminar flame zone of finite thickness. Both the Prandtl number and the Lewis number were assumed unity for this laminar boundary-layer flow model. The equations for conservation of energy, momentum and species were cast into a similar Blasius-type form. Both an exact numerical solution and an approximate solution were given.

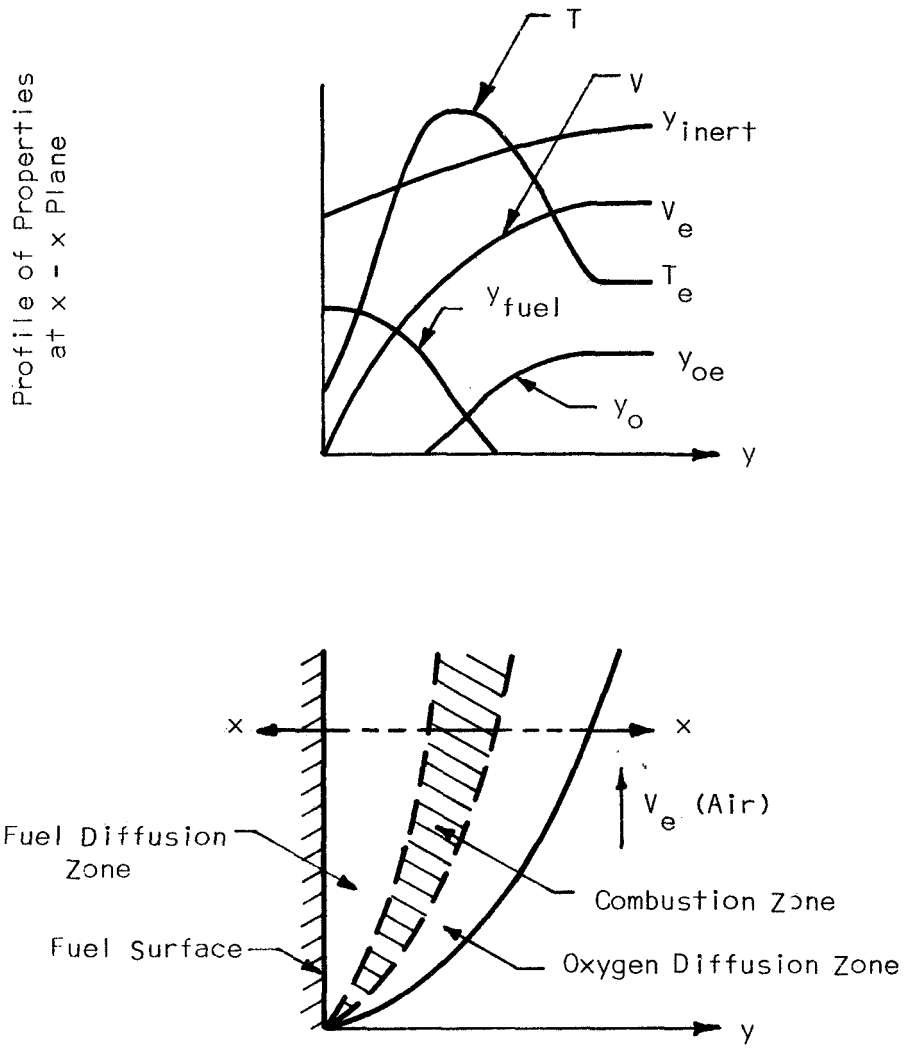


Figure II.2 Film Combustion Model of Emmons

By assuming chemical reaction occurs in an infinitesimally thin flame, i.e., with infinite chemical reaction rate, Toong (15) extended the work by Spalding and Emmons and obtained the velocity, temperature and composition profiles in the boundary layer along with combustion rates in the flame and at the fuel surface. This model was used later by Toong (16) to study the interaction mechanism between two parallel fuel plates.

The same approach was extended by Chen and Toong (17) to study the steady, laminar, boundary layer flow of an oxidizer over a two-dimensional wedge with mass transfer and combustion with an infinitesimally thin flame. The effects of the pressure gradient on skin friction, boundary layer separation and rates of evaporation and combustion were examined and discussed.

3. Turbulent Boundary Layer Model

Marxman and Gilbert (18) idealized the hybrid combustion problem by considering turbulent boundary layer flow over a flat plate. The turbulent diffusion flame front was assumed to be a surface of infinitesimal thickness, the position of which within the boundary layer was critical in determining the burning rate. Following the approach taken by Lees (19) in earlier turbulent boundary layer heat transfer studies, an expression for the mass burning rate was derived. This model represented the actual process quite well for a slow-burning Plexiglas-oxygen system according to Schlieren and shadowgraph photos taken by Muzzy (20).

Utilizing the integral technique of boundary layer theory, Marxman, Wooldridge and Muzzy (21) made a flame height analysis based on the model of Marxman and Gilbert (18) and developed a simplified equation for the

mass burning rate. The transient behavior caused by thermal lag in the solid fuel was discussed and an approximate expression for the transient burning rate of fuel was derived. Theoretically calculated flame positions and mass burning rates of fuel for flow over a flat plate were compared with measurements from a Plexiglas-oxygen slab burner. The regression rate equation as applied to a cylindrical tube was derived and compared with results from a tube burner. Good agreement was found in both cases.

By assuming that the chemical reaction rate is much greater than the local diffusion rate, Marxman (22) proposed a thin-flame model as shown in Figure II.3. Any chemical reaction was assumed to be confined to a thin-flame zone in the turbulent boundary layer. For the case of diffusion-limited combustion, the gas-phase mass, momentum and energy conservation equations for the steady, turbulent, boundary layer flow problem were solved with the mass flux from the solid fuel surface, $(\rho v)_w$, serving as a boundary condition. The generalized Reynolds analogy was assumed to be valid. Experimental verification of the above assumptions were reported by Wooldridge and Muzzy (23). A computer program for internal ballistic design of hybrid rockets has been developed based on this thin-flame model (24 - 26). Through comparisons with data on the Plexiglas-oxygen system, the capabilities and limitations of the thin-flame model were discussed (27).

B. Special Topics

Previous analytical treatment of hybrid rocket systems has been centered primarily on the development of regression rate equations. Limited work have been done to study the basic mechanisms involved in such systems.

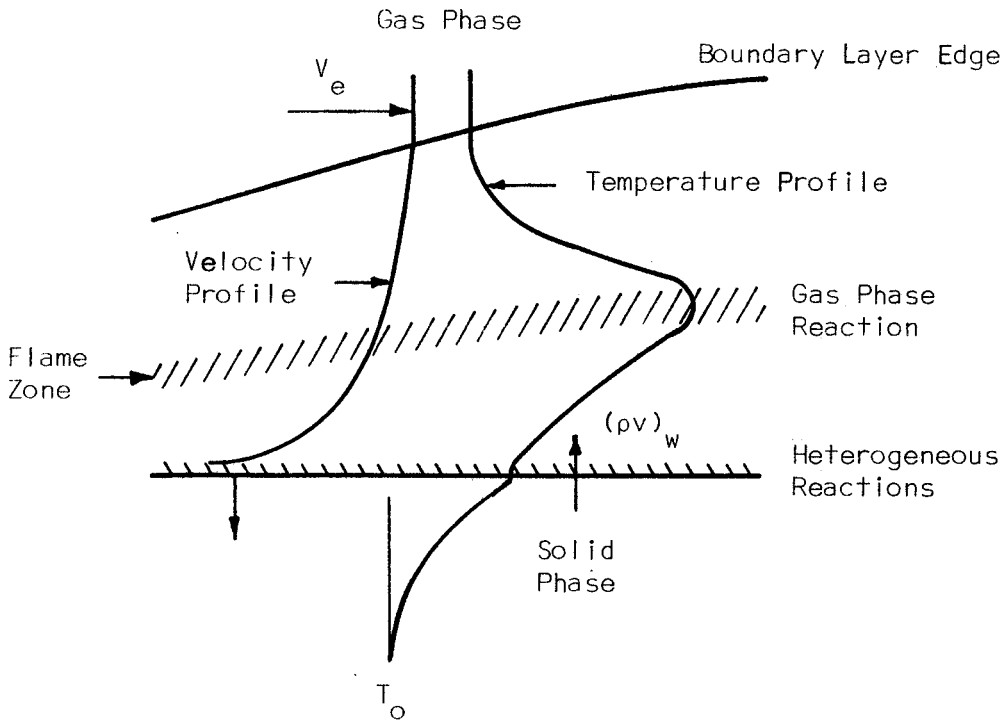


Figure II.3 Thin Flame Model of Marxman

The effects due to radiative heat transfer, variable fluid properties, chemical kinetics and transient behavior have been recognized as being important. Analytical work being done in these areas is discussed.

1. Radiative Heat Transfer

Fineman (4) was the first to recognize the importance of radiative heat transfer effects in hybrid rocket systems. A modified regression rate equation to account for radiative heat transfer effects has been developed by Marxman, Wooldridge and Muzzy (21). The radiative and convective heat-transfer mechanisms are found to be coupled. In the thin-flame theory, this modified regression rate equation can be used as one of the boundary conditions to account for radiative effects. Assuming a gray-body equilibrium description applies, a practical method to incorporate radiative effects in the analysis has been outlined (24, 25). The radiative heat transfer problem has received some attention, however, only a beginning towards an adequate description has been accomplished.

2. Variable Fluid Properties

A co-ordinate transformation related to the analogous Howarth-Dorodnitsyn transformation for laminar boundary layers has been adopted by Marxman (22) to relate the variable-property layer to an equivalent incompressible turbulent boundary layer. Such a transformation enables a description of the gross flow features through the evaluation of fluid properties at some reference state in the boundary layer. However, development of a semi-empirical expression for the reference state is needed.

3. Chemical Kinetics

The role of chemical kinetics in gas-phase combustion, solid-phase degradation and heterogeneous reaction at the gas-solid interface are topics of limited understanding. Treatment of the combustion process has been limited to the diffusion-controlled concept. Experimental investigations by Smoot and Price (10, 11) indicated that the diffusion-controlled concept is not adequate under certain conditions. The chemical kinetics of solid-phase degradation have been investigated by Houser and Peck (28) and by Rabinovitch (29) for the depolymerization process of unfilled polymers. Some theoretical investigations of the interaction between gas-phase kinetics, solid-phase kinetics and regression rate have been made recently by Marxman (27).

4. Transient Behavior

Although the transient behavior is considered to be very important in hybrid rocket systems, the subject has received little attention. The transient phenomena due to a sudden change in gas-phase heat transfer to the solid has been treated analytically (21). A limited experimental study of combustion instability has been reported (30, 31). A simple analysis of combustion instability due to low-frequency disturbances has been made, however, all previous analyses of the hybrid rocket system have been restricted by a quasi-steady state assumption.

CHAPTER III

MATHEMATICAL FORMULATION

In order to gain a basic understanding of the fundamental processes involved in hybrid rocket systems, a rather different approach from any of the previous analyses has been chosen. Instead of making a lot of simplifying assumptions to seek a closed-form solution, the current mathematical formulation is carried out with a view to take into account any effect that is considered to be important in hybrid rocket systems. Such an approach would allow a study of the relative importance of the various effects in question. Eventually, it is to be expected that the mathematical models can be used to simulate realistic experimental conditions.

First of all, a model for the physical system is defined. Mathematical models for the gas phase, the solid phase and the gas-solid interface are then formulated. The governing equations derived are expressed in dimensionless form. The variables that result from the formulation are classified.

A. Physical Model

Although present day computers have larger storage and higher speeds, it is still not practical to attempt a numerical solution of a transient, three-dimensional problem by means of computers. Hence, the physical system is restricted to a transient, two-dimensional one. The following assumptions are made for the physical system: (a) All dependent variables are symmetric with respect to the θ-direction in cylindrical co-ordinates, i.e., variation in the θ-direction is small compared to that in the radial

and the axial directions; (b) Non-receding fuel surface, i.e., effect due to a physically receding fuel surface is insignificant. A sketch of the physical system used is shown in Figure III.1.

B. Model for the Gas Phase

The gas phase in a hybrid rocket system generally consists of a nonisothermal multicomponent fluid of N chemical species. The general conservation equations for a multicomponent reacting gas mixture have been derived by Hirschfelder et. al. (32). Following the approach by Lees (33) and Chung (34) in formulating the equations for the mass, momentum and energy fluxes, a set of governing equations for the gas phase has been derived after some manipulations as follows:

Continuity Equation:

$$\frac{D\hat{\rho}}{D\hat{t}} + \hat{\rho}\left[\frac{\partial \hat{v}_r}{\partial \hat{r}} + \frac{\hat{v}_r}{\hat{r}} + \frac{\partial \hat{v}_z}{\partial \hat{z}}\right] = 0 \qquad \text{(III.1)}$$

Species Continuity Equations:

$$\hat{\rho}\frac{Dy_i}{D\hat{t}} = \frac{1}{ReSc}\left[\frac{\partial}{\partial \hat{r}}\left(\hat{\rho}\hat{D}_i \frac{\partial y_i}{\partial \hat{r}}\right) + \left(\frac{\hat{\rho}\hat{D}_i}{\hat{r}}\right)\left(\frac{\partial y_i}{\partial \hat{r}}\right) + \frac{\partial}{\partial \hat{z}}\left(\hat{\rho}\hat{D}_i \frac{\partial y_i}{\partial \hat{z}}\right)\right] + \frac{W_o r_o}{\rho_o v_o}\hat{W}_i$$

$$i = 1, 2, \ldots, N \qquad \text{(III.2)}$$

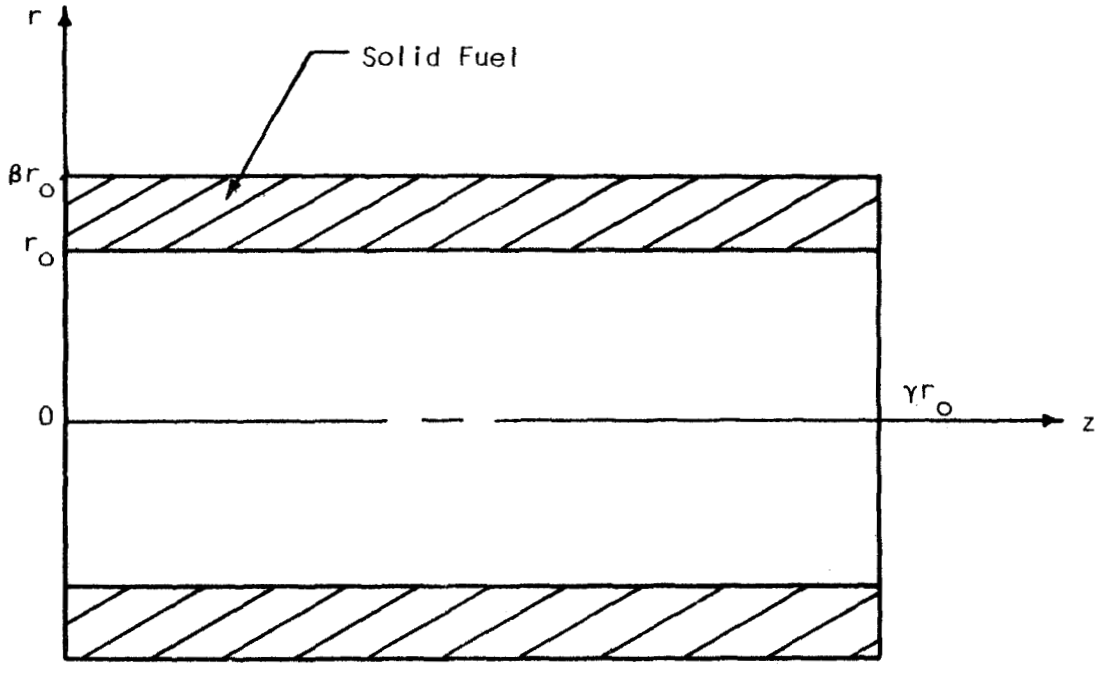


Figure III.1 Transient, Two-Dimensional, Reactive Fluid Flow in an "Idealized" Hybrid Rocket System

Momentum Equations:

$$\hat{\rho}\frac{D\hat{v}_r}{D\hat{t}} = -\frac{\partial\hat{P}}{\partial\hat{r}} + \frac{1}{Re}\left[\frac{2}{3}\frac{\partial}{\partial\hat{r}}\left\{\hat{\mu}\left(2\frac{\partial\hat{v}_r}{\partial\hat{r}} - \frac{\hat{v}_r}{\hat{r}} - \frac{\partial\hat{v}_z}{\partial\hat{z}}\right)\right\} + \frac{2}{3}\left(\frac{\hat{\mu}}{\hat{r}}\right)\left(2\frac{\partial\hat{v}_r}{\partial\hat{r}} - \frac{\hat{v}_r}{\hat{r}} - \frac{\partial\hat{v}_z}{\partial\hat{z}}\right) + \frac{\partial}{\partial\hat{z}}\left\{\hat{\mu}\left(\frac{\partial\hat{v}_z}{\partial\hat{r}} + \frac{\partial\hat{v}_r}{\partial\hat{z}}\right)\right\}\right]. \tag{III.3}$$

$$\hat{\rho}\frac{D\hat{v}_z}{D\hat{t}} = -\frac{\partial\hat{P}}{\partial\hat{z}} + \frac{1}{Re}\left[\frac{\partial}{\partial\hat{r}}\left\{\hat{\mu}\left(\frac{\partial\hat{v}_z}{\partial\hat{r}} + \frac{\partial\hat{v}_r}{\partial\hat{z}}\right)\right\} + \frac{\hat{\mu}}{\hat{r}}\left(\frac{\partial\hat{v}_z}{\partial\hat{r}} + \frac{\partial\hat{v}_r}{\partial\hat{z}}\right) + \frac{2}{3}\frac{\partial}{\partial\hat{z}}\left\{\hat{\mu}\left(2\frac{\partial\hat{v}_z}{\partial\hat{z}} - \frac{\partial\hat{v}_r}{\partial\hat{r}} - \frac{\hat{v}_r}{\hat{r}}\right)\right\}\right]. \tag{III.4}$$

Energy Equation:

$$\hat{\rho}\hat{C}_p\frac{D\hat{T}}{D\hat{t}} = Ec\frac{D\hat{P}}{Dt} + \frac{1}{PrRe}\left[\frac{\partial}{\partial\hat{r}}\left(\hat{\lambda}\frac{\partial\hat{T}}{\partial\hat{r}}\right) + \frac{\hat{\lambda}}{\hat{r}}\frac{\partial\hat{T}}{\partial\hat{r}} + \frac{\partial}{\partial\hat{z}}\left(\hat{\lambda}\frac{\partial\hat{T}}{\partial\hat{z}}\right)\right] + \frac{1}{ReSc}\left[\hat{\rho}\frac{\partial\hat{T}}{\partial\hat{r}}\left(\sum_i \hat{D}_i\hat{C}_{pi}\frac{\partial y_i}{\partial\hat{r}}\right) + \hat{\rho}\frac{\partial\hat{T}}{\partial\hat{z}}\left(\sum_i \hat{D}_i\hat{C}_{pi}\frac{\partial y_i}{\partial\hat{z}}\right)\right]$$

$$- \frac{r_o w_o}{\rho_o v_o}\left(\sum_i \hat{h}_i\hat{W}_i\right) \tag{III.5}$$

Equation of State:

$$\hat{P} = \frac{1}{Ec} \sum_{i=1}^{N} (y_i \hat{R}_i) \hat{\rho} \hat{T} \qquad (III.6)$$

where the operator, $\frac{D}{D\hat{t}}$, is defined as follows:

$$\frac{D}{D\hat{t}} \equiv \frac{\partial}{\partial \hat{t}} + \hat{v}_r \frac{\partial}{\partial \hat{r}} + \hat{v}_z \frac{\partial}{\partial \hat{z}} . \qquad (III.7)$$

The underlying assumption in deriving this set of governing equations are as follows:

(a) Flow of N-component gas mixture with chemical reactions,

(b) Isotropic, heterogeneous media,

(c) Gravity and external forces negligible,

(d) Newtonian fluid with negligible bulk viscosity, i.e., $\mu_B << \mu$,

(e) Fourier's law for heat conduction,

(f) System is a binary mixture so far as diffusion is concerned such that Fick's law for diffusion can be applied,

(g) Negligible viscous dissipation, radiative and Dufour effects,

(h) Ideal gas mixture such that enthalpy of the gas mixture can be defined as follows:

$$\hat{h} \equiv \sum_i (y_i \hat{h}_i) \qquad (III.8)$$

$$\hat{h}_i \equiv \int_1^{\hat{T}} \hat{C}_{pi} d\hat{T} + \hat{h}_{io} + \hat{h}_{Li} \qquad (III.9)$$

It has been pointed out by Bird et. al. (35) that equations (III.1 - III.2) constitute only N independent equations. For the numerical solution of this set of equations, it appears to be more convenient to eliminate equation (III.1). Hence, equations (III.2 - III.6) are the (N + 4) independent equations in the gas phase to be solved.

C. Model for the Solid Phase

The main concern in the solid phase is the temperature distribution. Hence, the governing equation in the solid phase is the familiar transient heat conduction equation as follows:

$$\hat{p}_s \hat{C}_s \frac{\partial \hat{T}_s}{\partial \hat{t}_s} = \frac{\alpha_{so}}{r_o v_o} \left[\frac{\partial}{\partial \hat{r}} \left(\hat{\lambda}_s \frac{\partial \hat{T}_s}{\partial \hat{r}} \right) + \frac{\hat{\lambda}_s}{\hat{r}} \left(\frac{\partial \hat{T}_s}{\partial \hat{r}} \right) + \frac{\partial}{\partial \hat{z}} \left(\hat{\lambda}_s \frac{\partial \hat{T}_s}{\partial \hat{z}} \right) \right. \qquad \text{(III.10)}$$

The restrictions are as follows:

(a) Isotropic, heterogeneous media,

(b) Fourier's law for heat conduction,

(c) No heat source or sink.

D. Model at the Gas-Solid Interface

A balance of mass and energy is assumed at the gas-solid interface at any instant of time based on the general conservation principle as follows:

$$\text{Out} - \text{In} = \text{Generated} \qquad \text{(III.11)}$$

The derived governing equations at the interface are shown as follows:

Mass Balance:

$$\frac{D_o}{r_o v_o}\left(\frac{\partial y_i}{\partial \hat{r}}\right)_w \hat{\rho}_w \hat{D}_{iw} - \hat{\rho}\hat{v}_w\, y_{iw} = \left(\frac{\rho_{so}}{\rho_o}\right)\left(\frac{\dot{r}_o}{v_o}\right)\hat{\rho}_s \hat{\dot{r}}\; y_{isw} \qquad i = 1, 2, \ldots, N$$

(III.12)

Energy Balance:

$$-\left(\frac{T_{so}}{T_o}\right)\left(\frac{\lambda_{so}}{\lambda_o}\right)\left(\hat{\lambda}_s \frac{\partial \hat{T}_s}{\partial \hat{r}}\right)_w = \hat{\rho}_w \hat{v}_w \left(\frac{r_o v_o}{\alpha_o}\right)\left\{\sum_i (\hat{h}_i y_i)_w\right\} - \left(\hat{\lambda}\frac{\partial \hat{T}}{\partial \hat{r}}\right)_w - \rho_w\left(\frac{D_o}{\alpha_o}\right)\left\{\sum_i \left(\hat{h}_i \hat{D}_i \frac{\partial y_i}{\partial \hat{r}}\right)_w\right\}$$

$$+ \hat{\rho}_{sw}\hat{\dot{r}}\left(\frac{T_{so}}{T_o}\right)\left(\frac{\lambda_{so}}{\lambda_o}\right)\left(\frac{r_o \dot{r}_o}{\alpha_{so}}\right)\left\{\sum_i (\hat{h}_{sg\ i} y_{isw})\right\} \qquad \text{(III.13)}$$

E. Classification of Variables

Since the physical model is a transient, two-dimensional problem, there are three independent variables, namely, $\hat{r}$, $\hat{z}$, and $\hat{t}$.

The governing equations in the gas phase consist of (N + 4) independent equations, and, there is one governing equation in the solid phase. Hence, a total of (N + 5) dependent variables can be solved by this set of governing equations. The dependent variables are $\hat{V}_r$, $\hat{V}_z$, $\hat{T}$, $\hat{T}_s$, $\hat{\rho}$ and y_i where i = 1, 2, ..., N.

The remaining variables can be expressed either as functions of the independent and/or the dependent variables, or, as constants. These variables are conveniently called functional variables. They are $\hat{P}$, $\hat{\mu}$, $\hat{D}_i$, $\hat{W}_i$, $\hat{\lambda}$, $\hat{C}_{pi}$, $\hat{C}_p$, $\hat{h}_i$, $\hat{h}_i{}^o$, $\hat{h}_{sg\ i}$, $\hat{\rho}_s$, $\hat{\lambda}_s$, $\hat{C}_s$ and $\hat{\dot{r}}$.

In normalizing the governing equations into dimensionless form, a number of dimensionless groups evolved. The values for these dimensionless groups depend on the characteristic values chosen for the problem. These values relate the relative importance of the various physical mechanisms involved in the system. The dimensionless groups are shown in Figure III.2.

Figure (III.2) Dimensionless Groups

$$Re \equiv \frac{r_o \rho_o v_o}{\mu_o} \qquad Sc \equiv \frac{\mu_o}{\rho_o D_o}$$

$$Pr \equiv \frac{C_{po} \mu_o}{\lambda_o} \qquad Ec \equiv \frac{v_o^2}{C_{po} T_o}$$

$$\frac{r_o w_o}{\rho_o v_o} \qquad \frac{D_o}{r_o v_o}$$

$$\frac{D_o}{\alpha_o} \qquad \frac{r_o v_o}{\alpha_o}$$

$$\frac{r_o v_o}{\alpha_{so}} \qquad \frac{r_o \dot{r}_o}{\alpha_{so}}$$

$$\frac{\rho_{so}}{\rho_o} \qquad \frac{T_{so}}{T_o}$$

$$\frac{\dot{r}_o}{v_o} \qquad \frac{\lambda_{so}}{\lambda_o}$$

CHAPTER IV

NUMERICAL SCHEMES

The governing equations derived in Chapter III can be solved numerically by the appropriate finite difference schemes. A choice of the numerical schemes is discussed. The selected numerical schemes are described.

A. Selection of Schemes

The governing equations in the gas phase can behave either as hyperbolic or parabolic partial differential equations depending on whether the first-order spatial derivatives or the second-order spatial derivatives are the dominating terms, respectively. For turbulent flow, i.e., Re > 2,000, the terms containing the second-order spatial derivatives are small compared with that of the first-order spatial derivatives. Hence, it has been decided that equations (III.2) through (III.5) are most likely to behave as first-order hyperbolic partial differential equations. The Lax-Wendroff centered difference scheme of second-order accuracy is commonly accepted as the standard finite difference scheme for the numerical solution of hyperbolic partial differential equations. Hence, the centered difference scheme is used to derive the difference equations for equations (III.2 - III.5).

Equation (III.10) is a parabolic partial differential equation. The Crank-Nicolson scheme is the most widely used finite difference scheme for solving this type of equation. It is, therefore, selected in deriving the difference equation for equation (III.10).

Equations (III.12) and (III.13) do not have time derivative term. It is only required that these equations be satisfied at any instant of time.

Thus, the difference equations for these equations are derived by using a time-independent finite difference scheme.

B. Lax-Wendroff Scheme

The Lax-Wendroff scheme is designed for the numerical solution of first-order hyperbolic partial differential equations. The finite difference analog for this scheme is centered between the time level and the spatial coordinates. The basic nature of this scheme and its applications are discussed by von Rosenberg (36). The nomenclature used and the center about which this numerical analog is based are presented schematically in Figure (IV.1). The second-order correct analogs for this centered difference scheme have been derived and are listed as follows:

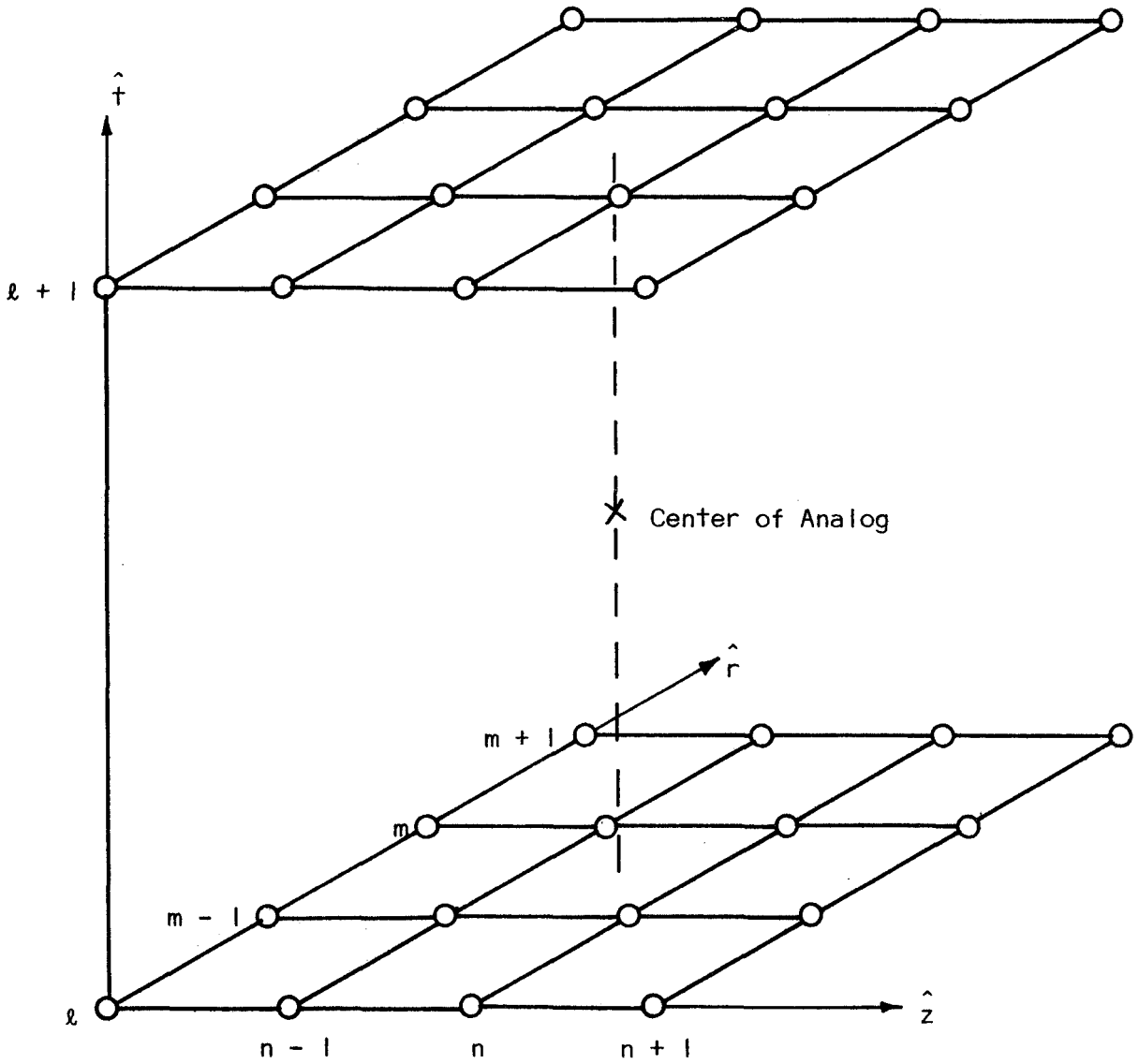


Figure IV.1 Lax-Wendroff Centered Difference Scheme

Analogs for Lax-Wendroff Scheme:

$$(r)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},\, n-\frac{1}{2}} \simeq (m - \tfrac{3}{2})(\Delta\hat{r})$$

$$(u)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},\, n-\frac{1}{2}} \simeq \frac{1}{8}\left[u^{\ell+1}_{m,n} + u^{\ell+1}_{m,n-1} + u^{\ell+1}_{m-1,n} + u^{\ell+1}_{m-1,n-1} + u^{\ell}_{m,n} + u^{\ell}_{m,n-1} + u^{\ell}_{m-1,n} + u^{\ell}_{m-1,n-1}\right]$$

$$\left(\frac{\partial u}{\partial \hat{t}}\right)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},n-\frac{1}{2}} \simeq \frac{1}{4(\Delta\hat{t})}\left[u^{\ell+1}_{m,n} + u^{\ell+1}_{m,n-1} + u^{\ell+1}_{m-1,n} + u^{\ell+1}_{m-1,n-1} - u^{\ell}_{m,n} - u^{\ell}_{m,n-1} - u^{\ell}_{m-1,n} - u^{\ell}_{m-1,n-1}\right]$$

$$\left(\frac{\partial u}{\partial \hat{r}}\right)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},n-\frac{1}{2}} \simeq \frac{1}{4(\Delta\hat{r})}\left[u^{\ell+1}_{m,n} + u^{\ell+1}_{m,n-1} - u^{\ell+1}_{m-1,n} - u^{\ell+1}_{m-1,n-1} + u^{\ell}_{m,n} + u^{\ell}_{m,n-1} - u^{\ell}_{m-1,n} - u^{\ell}_{m-1,n-1}\right]$$

$$\left(\frac{\partial u}{\partial \hat{z}}\right)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},n-\frac{1}{2}} \simeq \frac{1}{4(\Delta\hat{z})}\left[u^{\ell+1}_{m,n} - u^{\ell+1}_{m,n-1} + u^{\ell+1}_{m-1,n} - u^{\ell+1}_{m-1,n-1} + u^{\ell}_{m,n} - u^{\ell}_{m,n-1} + u^{\ell}_{m-1,n} - u^{\ell}_{m-1,n-1}\right]$$

Analogs for Lax-Wendroff Scheme (continue):

$$\left(\frac{\partial^2 u}{\partial \hat{r}^2}\right)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},n-\frac{1}{2}} \simeq \frac{1}{8(\Delta r)^2}\Big[u^{\ell+1}_{m+1,n} + u^{\ell+1}_{m+1,n-1} - u^{\ell+1}_{m,n} - u^{\ell+1}_{m,n-1} - u^{\ell+1}_{m-1,n} - u^{\ell+1}_{m-1,n-1} + u^{\ell+1}_{m-2,n} + u^{\ell+1}_{m-2,n-1}$$

$$+ u^{\ell}_{m+1,n} + u^{\ell}_{m+1,n-1} - u^{\ell}_{m,n} - u^{\ell}_{m,n-1} - u^{\ell}_{m-1,n} - u^{\ell}_{m-1,n-1} + u^{\ell}_{m-2,n} + u^{\ell}_{m-2,n-1}\Big]$$

$$\left(\frac{\partial^2 u}{\partial \hat{z}^2}\right)^{\ell+\frac{1}{2}}_{m-\frac{1}{2},n-\frac{1}{2}} \simeq \frac{1}{8(\Delta \hat{z})^2}\Big[u^{\ell+1}_{m,n+1} - u^{\ell+1}_{m,n} - u^{\ell+1}_{m,n-1} + u^{\ell+1}_{m,n-2} + u^{\ell+1}_{m-1,n+1} - u^{\ell+1}_{m-1,n} - u^{\ell+1}_{m-1,n-1} + u^{\ell+1}_{m-1,n-2}$$

$$+ u^{\ell}_{m,n+1} - u^{\ell}_{m,n} - u^{\ell}_{m,n-1} + u^{\ell}_{m,n-2} + u^{\ell}_{m-1,n+1} - u^{\ell}_{m-1,n} - u^{\ell}_{m-1,n-1} + u^{\ell}_{m-1,n-2}\Big]$$

C. Crank-Nicolson Scheme

The Crank-Nicolson scheme is generally used for the numerical solution of second-order parabolic partial differential equations. The finite difference analog for this scheme is centered between the time level and at the particular spatial coordinate point in question. A very thorough discussion of this scheme and its applications can be found in Reference (36). The nomenclature used and the center about which this numerical analog is based are presented schematically in Figure (IV.2). The second-order correct analogs for this centered difference scheme have been derived and are listed as follows:

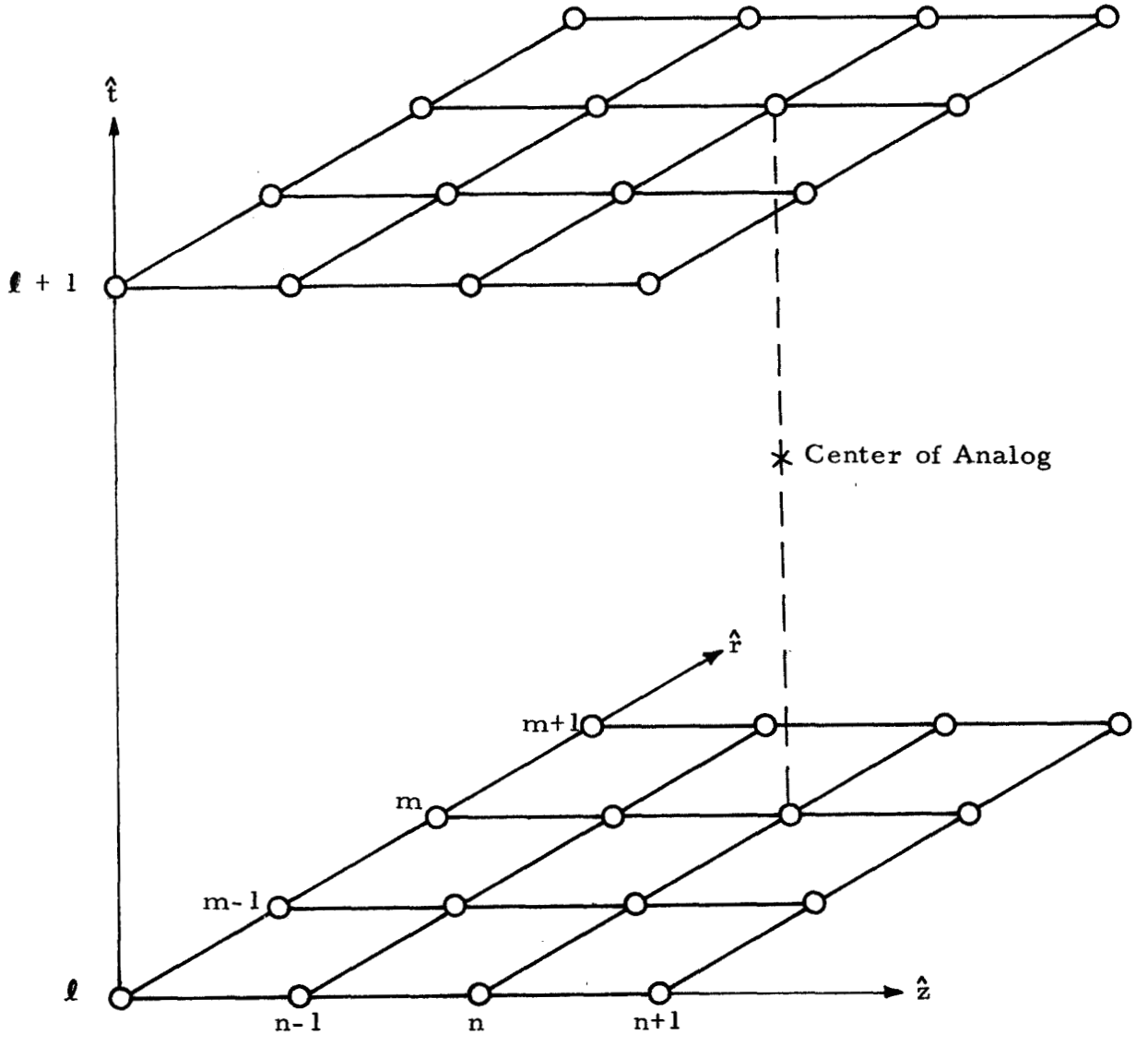


Figure IV.2 Crank-Nicolson Scheme

Analogs for Crank-Nicolson Scheme:

$$(\hat{r})_{m,n}^{\ell+\frac{1}{2}} \simeq m(\Delta\hat{r})$$

$$(u)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{2}\left[u_{m,n}^{\ell+1} + u_{m,n}^{\ell}\right]$$

$$\left(\frac{\partial u}{\partial \hat{t}}\right)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{\Delta\hat{t}}\left[u_{m,n}^{\ell+1} - u_{m,n}^{\ell}\right]$$

$$\left(\frac{\partial u}{\partial \hat{r}}\right)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{4(\Delta\hat{r})}\left[u_{m+1,n}^{\ell+1} + u_{m+1,n}^{\ell} - u_{m-1,n}^{\ell+1} - u_{m-1,n}^{\ell}\right]$$

$$\left(\frac{\partial u}{\partial \hat{z}}\right)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{4(\Delta\hat{z})}\left[u_{m,n+1}^{\ell+1} + u_{m,n+1}^{\ell} - u_{m,n-1}^{\ell+1} - u_{m,n-1}^{\ell}\right]$$

$$\left(\frac{\partial^2 u}{\partial \hat{r}^2}\right)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{2(\Delta\hat{r})^2}\left[u_{m+1,n}^{\ell+1} + u_{m+1,n}^{\ell} - 2u_{m,n}^{\ell+1} - 2u_{m,n}^{\ell} + u_{m-1,n}^{\ell+1} + u_{m-1,n}^{\ell}\right]$$

$$\left(\frac{\partial^2 u}{\partial \hat{z}^2}\right)_{m,n}^{\ell+\frac{1}{2}} \simeq \frac{1}{2(\Delta\hat{z})^2}\left[u_{m,n+1}^{\ell+1} + u_{m,n+1}^{\ell} - 2u_{m,n}^{\ell+1} - 2u_{m,n}^{\ell} + u_{m,n-1}^{\ell+1} + u_{m,n-1}^{\ell}\right]$$

D. Difference Scheme for Boundary Equations

At the interface, the governing equations involve only first-order spatial derivatives in the radial direction. Since no time derivative is involved, a common finite difference scheme for ordinary differential equations is sufficient for the numerical solution of these equations. A second-order correct analog compatible with those of the Lax-Wendroff and Crank-Nicolson schemes is chosen to approximate the radial derivative at the interface. The radial derivative at the interface is approximated as follows:

$$\left(\frac{\partial u}{\partial \hat{r}}\right)^{\ell}_{\frac{1}{2},n} \simeq \frac{u^{\ell}_{1,n} - u^{\ell}_{o,n}}{(\Delta \hat{r})} . \qquad \text{(IV.1)}$$

CHAPTER V

NUMERICAL ANALYSIS

The appropriate finite difference analogs derived in Chapter IV are substituted into the appropriate governing equations derived in Chapter III to obtain a set of linear independent equations. Numerical checkout of these difference equations has been performed. Since the numerical schemes are implicit, iterative procedures have to be used. These highly-coupled equations are very slowly convergent in nature, therefore, it has been found necessary to employ both a relaxation procedure and an accelerated convergence procedure during iterations at each time level. The reduction of roundoff errors and the convergence criteria used are discussed.

A. Numerical Checkout

When the governing partial differential equations are replaced by a finite difference equations, it is necessary to perform a numerical checkout to ascertain that no error has been introduced in the replacement process. The checkout procedure is described in the following paragraph.

A value equal to unity is assigned to all the variables. Values calculated by computer are checked against independent hand calculations for these finite difference equations. Any error found is then corrected. A value equal to zero is assigned to certain variables while the remaining variables are still unity. Computer and hand calculations are performed and the necessary corrections are made. This process is repeated by assigning a value equal to zero to some of the variables and unity to the

remaining variables. Through careful planning in selecting the value zero or unity for the variables, the process is continued until one is reasonably certain that no error remains.

Analytical solutions for the steady-state, two-dimensional heat conduction problem generally exist. The transient heat conduction equation can be verified by comparing its steady-state results with those from an analytical solution. By this means, the verification of Equation (III.10) has been performed and the detail is included in Appendix A. A maximum error of 2.1% has been calculated. This added more confidence in the numerical checkout procedure and the accuracy of the remaining difference equations.

B. Relaxation Procedure

It has been found that the boundary equations tend to diverge when a straight forward iteration procedure is used. Hence, a commonly used relaxation procedure is incorporated. Basically, this relaxation procedure assumes that the newly guessed value, u_{j+1}, for any of the dependent variables is linearly dependent on both the previously guessed value, u_j, and the value calculated by the difference equation, $f(u_j)$. Mathematically, this relaxation procedure can be expressed as follows:

$$u_{j+1} = \varepsilon u_j + (1 - \varepsilon) f(u_j) \qquad \text{(V.1)}$$

where ε is any number between zero and unity. In order to avoid instability, a very conservative value for ε should be selected. Thus, a value equal to 0.9 has been chosen for ε.

C. Aitken's δ^2-Method

The Aitken's δ^2-method is an explicit iteration procedure for the iterative solutions of non-linear equations. It is used to convert any convergent sequence (no matter how generated), $\{u_j\}$, into a more rapidly convergent sequence, $\{u_j'\}$, by using the following equation:

$$u_j' = u_j - \frac{(u_{j+1} - u_j)^2}{u_{j+2} - 2u_{j+1} + u_j} . \qquad (V.2)$$

A very detailed discussion of this method and the mathematical proof are given by Isaacson and Keller (37). This functional iteration scheme can accelerate the convergence by taking only $\frac{1}{2}$ of the iterations previously required or even better. A numerical example to demonstrate this accelerated convergence procedure is given by Henrici (38).

D. Roundoff Errors

Roundoff errors are inevitable when computations are carried out by computers. An introduction to the analysis of roundoff errors involved in the arithmetic operations of modern, high-speed computers has been given by Wilkinson (39). Since fourteen significant figures are stored for any floating point variable on the CDC6600 computer, the roundoff errors due to arithmetic operations on the CDC6600 computer can generally be ignored. However, the solution of the difference equations involves additions and subtractions of a very large number of terms which are significantly different in their order of magnitude. It is, therefore, believed that roundoff errors may play an important role in the numerical solution of these difference equations.

There is no general rule as to how addition and subtraction should be carried out in order to minimize roundoff errors. However, intuitively, one would expect that roundoff errors could be minimized if addition and subtraction were carried out such that in each operation the resulting change were a minimum. Thus, an analysis of the order of magnitude of the various terms in the difference equations has been made. Terms of the same order of magnitude are grouped together. Starting from the lowest order of magnitude term, addition and/or subtraction is carried out with the next higher order of magnitude term and so on. It has been found that such a grouping of terms has reduced the roundoff errors so significantly that the critical time increment is improved by at least two orders of magnitude.

E. Convergence Criteria

Convergence criteria are generally selected to suit the type of numerical problem to be solved. Values for the radial velocity component and the mass fraction of fuel at certain grid points can be so small that they are practically equal to zero. Thus, this should be taken into account in selecting the convergence criteria. It has been decided that the convergence criteria used should require that any one of the dependent variables at any grid point satisfy a certain predetermined tolerance, ζ, and that the sum of the relative error of any one of the dependent variables over all the grid points be smaller than a certain predetermined value, η. Mathematically, the convergence criteria used can be expressed as follows:

$$|f(u_j) - u_j| \leq \zeta \tag{V.3}$$

and,

$$\sum_{\substack{\text{over all} \\ \text{grid points}}} \frac{|f(u_j) - u_j|}{u_j} \leq \eta. \tag{V.4}$$

CHAPTER VI

SOLUTION FOR A SIMPLE CASE

In order to gain insight into the numerical problems and computational power involved, it was decided to solve a simple case. A one-step overall irreversible gas phase reaction is assumed, e.g., fuel + oxidizer → product, such that the number of chemical species present in the gas phase is a minimum, i.e., N = 3. The fuel and the oxidizer are selected. Models for the properties, the regression rate and the chemical reaction are formulated. A favorable downstream pressure gradient is imposed to correspond to a realistic physical situation. The boundary and initial conditions are defined. The selection of thermochemical and transport properties are discussed and the choice of physical parameters are outlined.

A. Selection of Fuel and Oxidizer

Lithium, beryllium, boron and aluminum are the light metals whose large heats of combustion have made them attractive as chemical propellants (40). When these light metals react with oxygen, it appears that only beryllium and aluminum form stable liquid oxides. Since beryllium is toxic, aluminum can be considered as, potentially, the most desirable chemical propellant available. In previous work, aluminum has been widely used as an additive fuel in experimental hybrid rocket systems (41, 42). McAlevy *et. al.* (43) have selected the aluminum-oxygen system in their study of the combustion of porous-metal hybrid rocket system. Hence, it has been decided to select aluminum as the fuel, oxygen as the oxidizer

and aluminum oxide as the product.

B. Model for Properties

The properties, in general, are strongly dependent on temperature. For the current solution, however, constant properties are assumed. The underlying assumptions are as follows:

(a) Constant transport properties by using equivalent turbulent values, i.e.,

$$\hat{\mu} = \text{constant}, \tag{VI.1}$$

$$\hat{D}_i = \text{constant}, \tag{VI.2}$$

$$\hat{\lambda} = \text{constant}; \tag{VI.3}$$

(b) Constant fluid properties, i.e.,

$$\hat{C}_{pi} = \text{constant}, \tag{VI.4}$$

$$\hat{h}_i^{\,o} = \text{constant}, \tag{VI.5}$$

$$\hat{h}_{sgi} = \text{constant}; \tag{VI.6}$$

(c) Constant properties for solid fuel, i.e.,

$$\hat{\rho}_s = \text{constant}, \tag{VI.7}$$

$$\hat{\lambda}_s = \text{constant}, \tag{VI.8}$$

$$\hat{C}_s = \text{constant}. \tag{VI.9}$$

C. Model for the Regression Rate of Fuel

The regression rate of fuel has been the main concern in previous analyses of hybrid rocket systems. Since the current objective is to test out the numerical solution proposed, a simplified model for the regression rate of fuel is used. While the position of the fuel surface is assumed to be fixed, to be consistent with the non-receding fuel surface assumption made for the physical system, mass addition of fuel from the fuel surface is assumed. Physically, this corresponds to the case where mass of fuel is added to the flow stream through a porous wall. It is further assumed that the rate of mass addition from the fuel surface is a constant, i.e.,

$$\hat{\dot{r}} = \text{constant}. \qquad \text{(VI.10)}$$

A study of the effect due to a variable rate of mass addition from the fuel surface is proposed in Chapter IX.

D. Model for Chemical Reaction

A semi-empirical approach has been adopted to describe the finite-rate chemical reaction in the gas phase. The assumptions made are described as follows:

(1) The gas-phase chemical reaction can be represented by a single overall irreversible chemical reaction, such as, fuel + oxidizer → product. According to Wilson (44), the gas-phase chemical reaction for aluminum-oxygen system is as follows:

$$2Al + \frac{3}{2} O_2 \rightarrow Al_2O_3(\ell). \qquad (VI.11)$$

(2) When the fuel-oxidizer ratio is within the flammability limits, the rate of production of species for this overall reaction is calculated in the same manner as for an elementary chemical reaction as follows:

$$\hat{W}_i = \frac{M_i}{W_o} (\nu_i'' - \nu_i')k \prod_{j=1}^{N} \left(\frac{\rho y_i}{M_j}\right)^{\nu_j'} \qquad (VI.12)$$

where ν_i' and ν_i'' are the stoichiometric coefficients for species, i, appearing as a reactant and as a product respectively. Species which are not reactants will have $\nu_i' = 0$, while those which do not appear as products have $\nu_i'' = 0$.

(3) The specific reaction-rate coefficient or rate constant is estimated from collision theory. For bimolecular reaction, the rate constant, k, can be estimated as follows (45):

$$k = S\sigma_{12}^2 \left[\left(\frac{8\pi RT(M_1 + M_2)}{M_1M_2}\right)\right]^{\frac{1}{2}} \exp\left[\frac{E}{RT}\right] \qquad (VI.13)$$

where S is the steric factor, σ_{12} is the average diameter of colliding species and E is the activation energy.

E. Imposed Pressure Gradient

The static pressure over the entire flow field has to be specified to correspond to a realistic physical situation so that a unique numerical solution can be obtained. Jones and Isaacson (46) have found experimentally

that both mass injection and combustion increase the axial pressure gradient. It is, therefore, necessary to obtain transient static pressure data in order that the numerical solution can be realistic. Since such experimental data are not available, the current solution imposes a constant favorable downstream pressure gradient equal to that used by Jones and Isaacson (46) in their analysis so that qualitative comparison of results can be made.

F. Initial and Boundary Conditions

The assumptions are as follows:

(a) Flow of the gaseous oxidizer is accelerated to a given initial velocity with mass addition from the solid fuel surface;

(b) The initial axial component of velocity distribution is based on the $(\frac{1}{7})$-power law for turbulent flow, i.e.,

$$\hat{v}_z = (1 - \hat{r})^{1/7}; \qquad \text{(VI.14)}$$

(c) The initial temperature profile corresponds to the conditions when ignition has just been completed.

(d) Inlet conditions and temperatures at the boundary surface of the solid fuel are constant;

(e) The axial component of velocity is zero at the interface and the radial component of velocity is required to be zero at the center line.

G. Selection of Thermochemical and Transport Properties

Since the current models for properties are too crude to represent

the actual physical situation, no emphasis has been placed on the accuracy of the values chosen for the properties. Whenever the value for a property is not directly available, its value is estimated.

The viscosity of the gas mixture due to molecular transport can be estimated by following one of the methods outlined by Bird et. al. (35) to be 0.00004 lb_m/sec/ft. The eddy viscosity distribution of a fully established turbulent flow through a pipe has been measured experimentally by Rothfus et. al. (47). An average value for the eddy viscosity across a pipe is estimated to be approximately 20 times that due to molecular transport. Hence, a value equal to 0.0008 lb_m/sec/ft is selected for μ. Assuming that the turbulent transports of mass, momentum and energy are similar and equal, the binary diffusion coefficient and the thermal conductivity are chosen such that $Sc \simeq 1$ and $Pr \simeq 1$, respectively. Hence, these selected values are D_i = 0.00592 ft^2/sec and λ = 1.2 Btu/hr/ft/°R.

The selected thermophysical properties for aluminum, oxygen, and aluminum oxide are tabulated as shown in Table (VI.1). These data are obtained either directly or by estimation from references (48) through (52).

From reference (52), the values for aluminum in the solid phase are selected as follows:

$$\rho_s = 168.5 \ lb_m/ft^3, \qquad (VI.15)$$

$$\lambda_s = 122.0 \ Btu/hr/ft/°R, \qquad (VI.16)$$

$$C_s = 0.221 \ Btu/lb_m/°R. \qquad (VI.17)$$

Table (VI.1) Selected Thermophysical Properties for Aluminum, Oxygen and Aluminum Oxide

	$Al(g)$	$O_2(g)$	$Al_2O_3(\ell)$
M, lb_m/mole	26.98 (48)	32.0 (48)	101.96 (48)
C_p, Btu/lb_m	0.26 (49)	0.295(50)	0.27 (51)
$h°$, Btu/lb_m	0	0	-7110.0 (52)
Boiling point, °R	4932.3 (52)	162.34 (48)	6840.0 (52)
$h_{s\ell}$, Btu/lb_m	170.0 (52)	-	510.0 (52)
$h_{\ell g}$, Btu/lb_m	4710.0 (52)	-	2590.0 (52)

Experimental data on the regression rates of various metalized hybrid fuel systems were reviewed (11, 24). It has been decided to choose a value in the order of 0.01 in/sec for the regression rate of fuel for consistency with the non-receding fuel model. The regression rate of aluminum is selected as

$$\dot{r} = 0.0008 \text{ ft/sec.} \qquad \text{(VI.18)}$$

It does not appear that the limits of flammability for the gas phase aluminum-oxygen reaction have been published in the open literature. The flammability limits for hydrocarbon fuels with air collected by Barnett and Hibbard (53) are reviewed. Values of 0.5 and 3.5 have been arbitrarily selected for the lean and rich limits of flammability, expressed as the fuel-oxidizer ratio to the stoichiometric fuel-oxidizer ratio, for the aluminum-oxygen system respectively.

The average diameter of colliding species, σ_{12}, can be expressed as the sum of the effective radius of the colliding aluminum atom and oxygen molecule. For aluminum, the effective radius is its atomic radius. A value of 1.43 Å is given by Bassow (54). For the oxygen molecule, the effective diameter can be approximated by the characteristic diameter based on the Lennard-Jones potential function. A value of 3.43 Å is given by Hirschfielder et. al. (32).

From the collision theory, the steric factor is the probability that a colliding pair will be oriented favorably for reaction. Hence, it should be a number equal to or less than unity. Newhall (55) has pointed

out that the steric factor is really an empirical correction factor to force the theoretical model to fit the experimental data. Since experimental data on aluminum-oxygen gas phase reaction are not available, a value equal to unity is chosen for the steric factor.

Semi-empirical expressions have been developed by Hirschfelder (56) for the calculations of activation energies of exothermic gas phase reactions of the form $a + bc \rightarrow ab + c$ and $ab + cd \rightarrow ac + bd$. The aluminum-oxygen gas phase reaction is quite complex. A review of the data collected in reference (56) indicated that the activation energies for the more complex gas phase reactions are in the range of 40-60 kcal/g-mole. Thus, a value of 50 kcal/g-mole is arbitrarily chosen for the aluminum-oxygen gas phase reaction.

H. Choice of Physical Parameters

Although values for physical parameters such as chamber radius, chamber pressure, flow velocity, etc., can be selected more freely, the following restrictions should be observed: (a) values chosen should be realistic, (b) the Mach number should be small, (c) the Reynolds number should have a value corresponding to turbulent flow. Values selected for the physical parameters are

$$r_o = 0.25 \text{ ft} \tag{VI.19}$$

$$r_e = 0.2875 \text{ ft} \tag{VI.20}$$

$$L = 0.09 \text{ ft} \tag{VI.21}$$

$$P = 10 \text{ atmosphere} \tag{VI.22}$$

$$v_o = 20 \text{ ft/sec.} \tag{VI.23}$$

CHAPTER VII

RESULTS FROM COMPUTER CALCULATION

A computer program has been developed to study the transient phenomena of reactive fluid flow in a hybrid rocket system. A detailed description of this computer program and its capability are included in Appendix B as computer program HETCOMB.

A separate computer program is employed to present the results calculated from computer program HETCOMB in graphical form. The usage of this plotting program and its options are described in Appendix C as computer program PLOT.

In order to conserve computational time, rather course grid spacings are chosen for the numerical calculation. There are, totally, 10 axial points, 20 radial points in the gas phase and 15 radial points in the solid phase. The detail of the grid points used is presented in Figure VII.1.

Initial values are assigned to all the dependent variables to correspond to the initial and boundary conditions described in Chapter VI. It has been found that the energy balance equation at the interface is inadequate to describe the physical mechanisms involved. When the initial temperature profile in the solid phase is chosen such that the transient temperature variation in the solid phase can be studied, a relatively low temperature value at the interface is calculated by the energy balance equation. This problem, presumably, can be eliminated if an additional energy production term due to radiative heat transfer

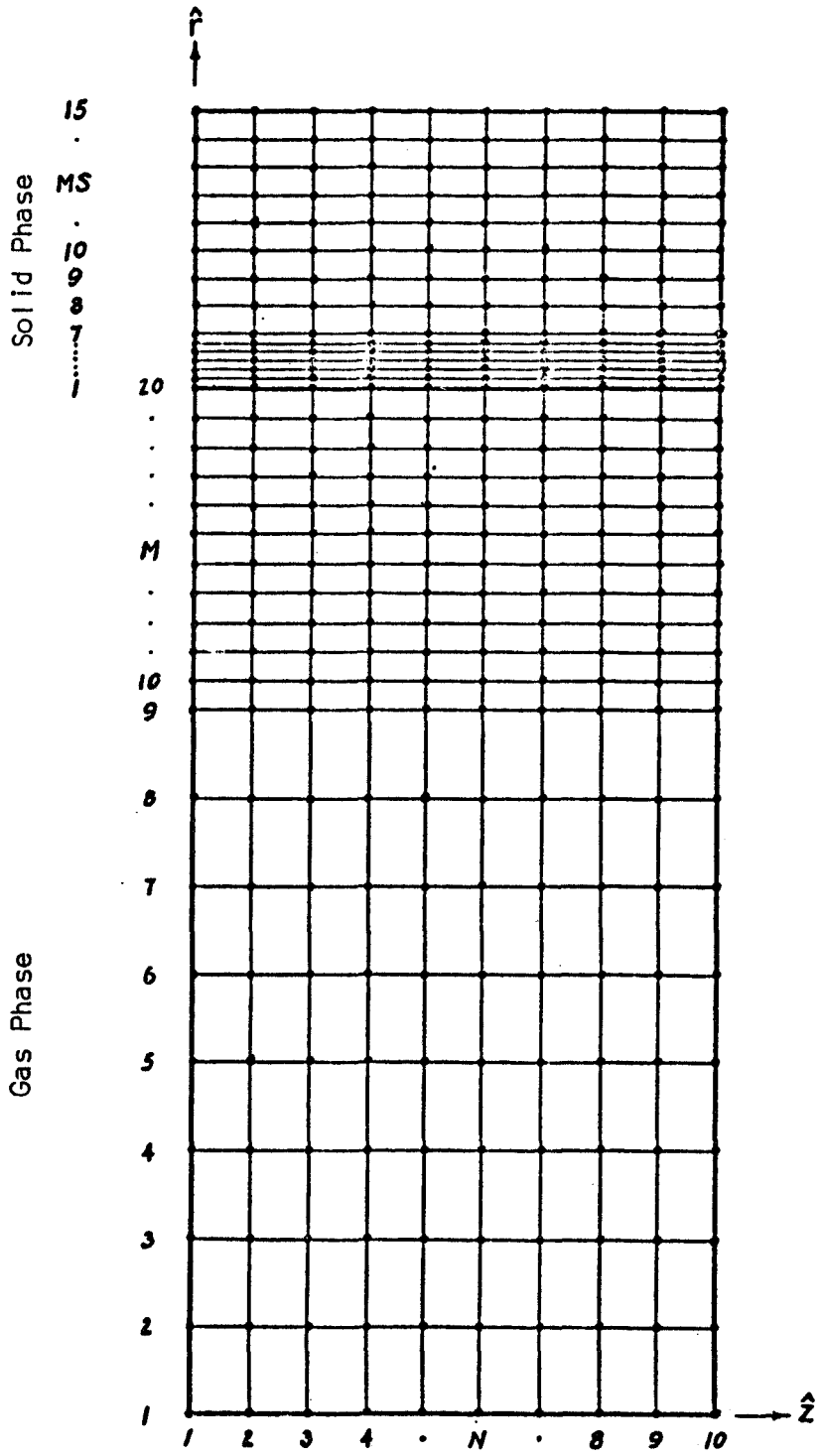


Figure VII.1 Grid Points Used for the Finite Difference Approximation

is included in the energy balance equation. Hence, the effect due to radiative heat transfer should definitely be incorporated in future work. In the mean time, in order to maintain a realistic temperature value at the interface, a steady-state temperature profile in the solid phase is assumed at the start of the combustion process. Initial profiles of the 8 dependent variables, $\hat{\rho}$, $\hat{v}_r$, $\hat{v}_z$, $\hat{T}$, y_{Al}, y_{O_2}, $y_{Al_2O_3}$ and $\hat{T}_s$, at any axial position are plotted as shown in Figure VII-2.1 - VII-2.8.

In order to start the iteration process, all the dependent variables at the first time level have to be assigned certain values. For convenience, the dependent variables at the first time level have been assigned the corresponding initial values at time equal to zero.

Numerical calculations for the simple case as outlined in Chapter VI were performed on the CDC6600 computer. With $\zeta = 0.01$ and $\eta = 0.01$ as the convergence criteria, the critical time increment was determined empirically to be in the range of 3 - 6 microseconds. With $\Delta t \simeq 3$ microseconds, numerical calculations were performed with $\zeta = 0.01$ and $\eta = 0.01$ for 1000 time steps. Tightening the convergence criteria by reassigning a value of 0.005 for η, numerical calculations were continued for another 1000 time steps. With $\eta = 0.002$, another 1000 time steps calculations were performed and a steady-state solution was reached at the end of 3000 time steps. The calculated results from computer program HETCOMB are presented in graphical form through the use of computer program PLOT.

Figure VII-2.1 - VII-2.8 Initial Profile of All the Dependent Variables at Any Axial Position

FIGURE (VII-2.1)
INITIAL PROFILE IN GAS PHASE

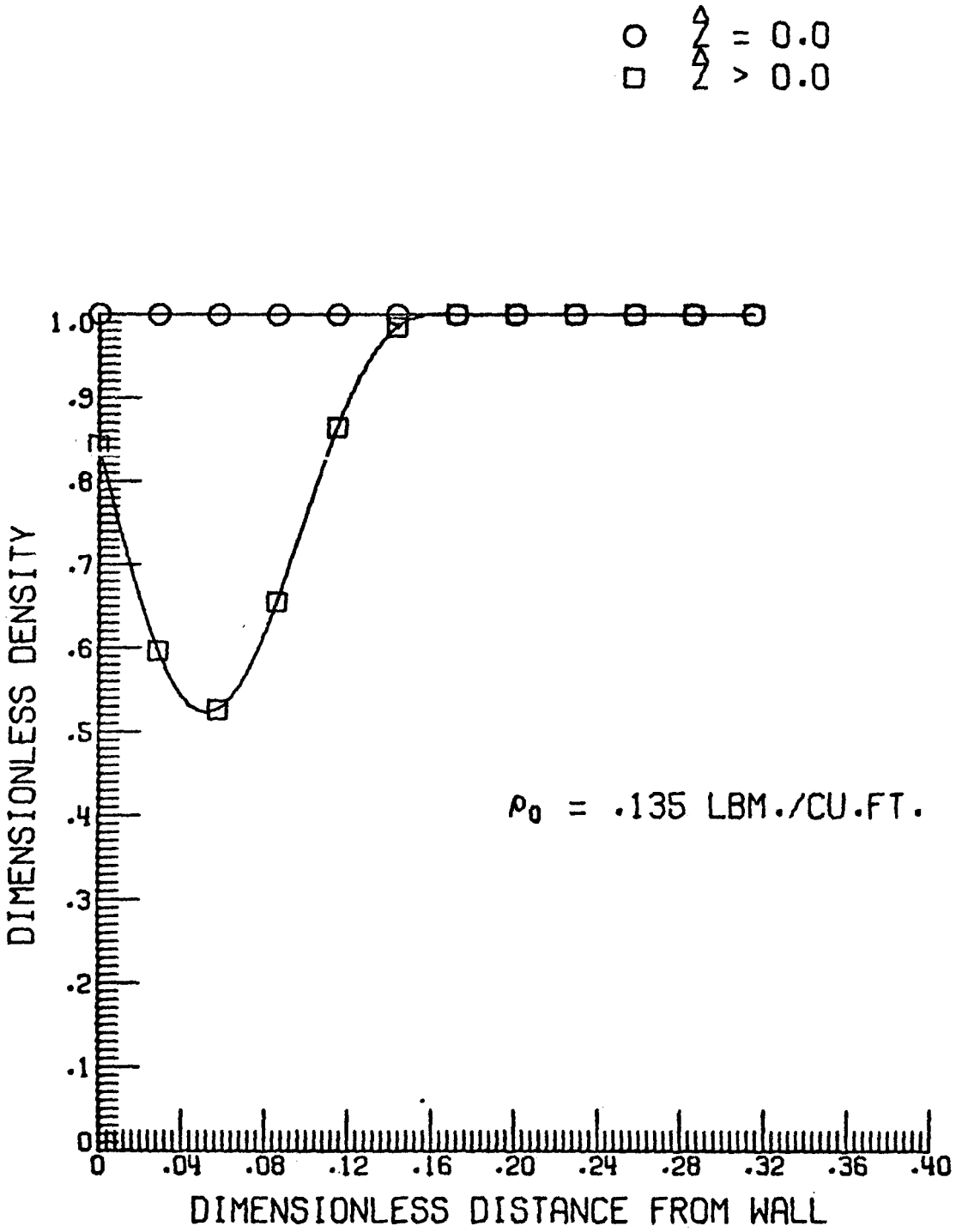


FIGURE (VII-2.2)
INITIAL PROFILE IN GAS PHASE

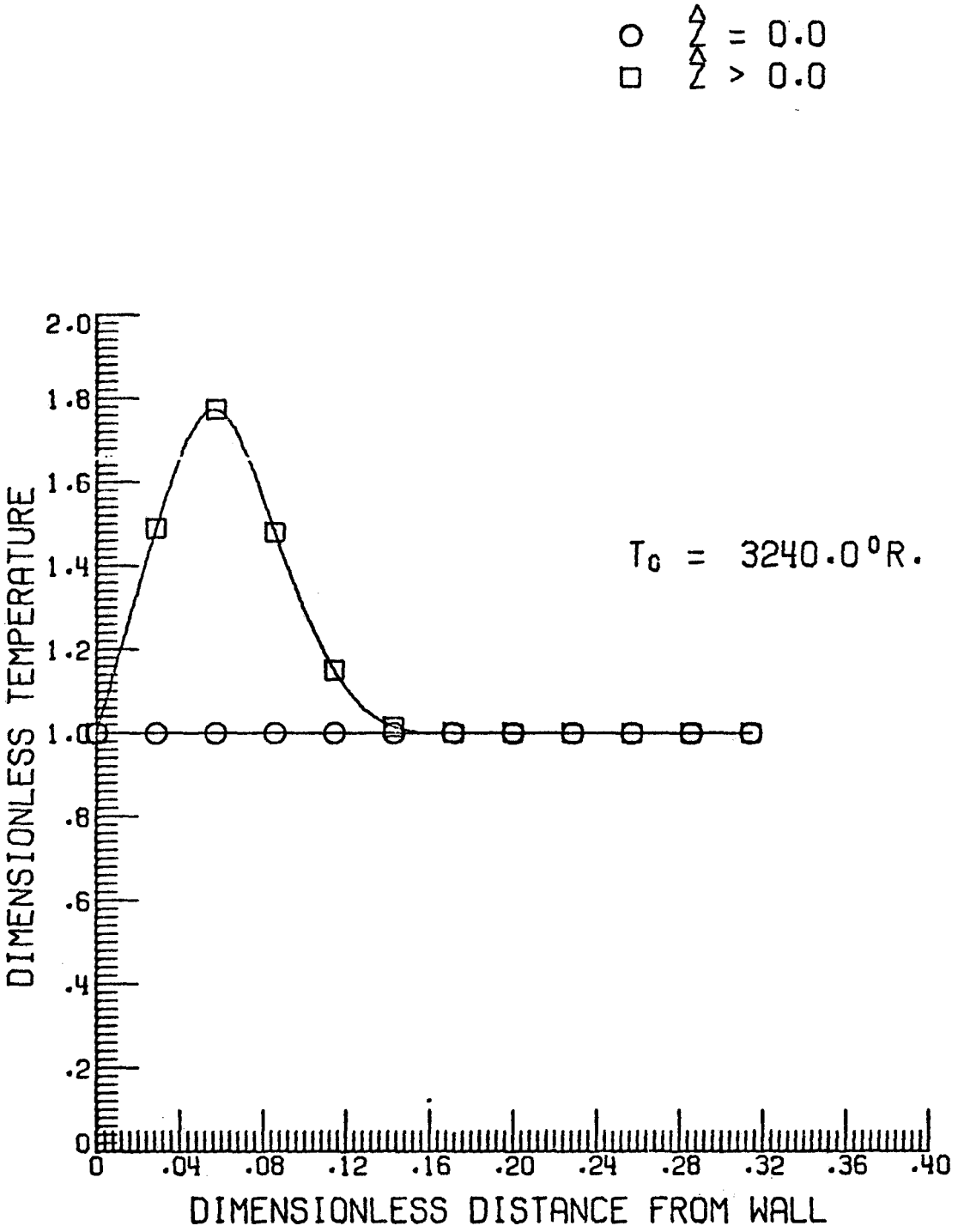


FIGURE (VII-2.3)
INITIAL PROFILE IN GAS PHASE

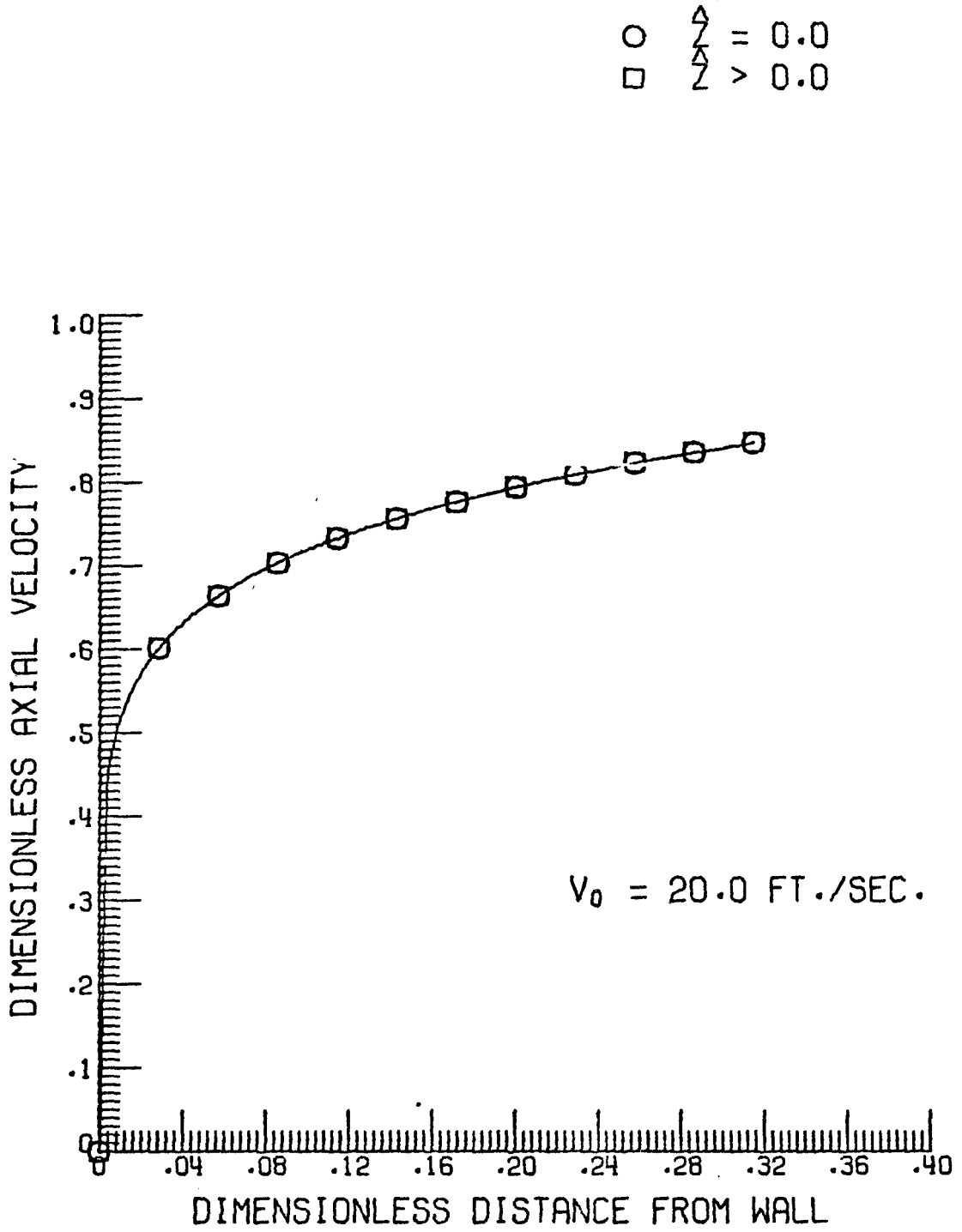


FIGURE (VII-2.4)
INITIAL PROFILE IN GAS PHASE

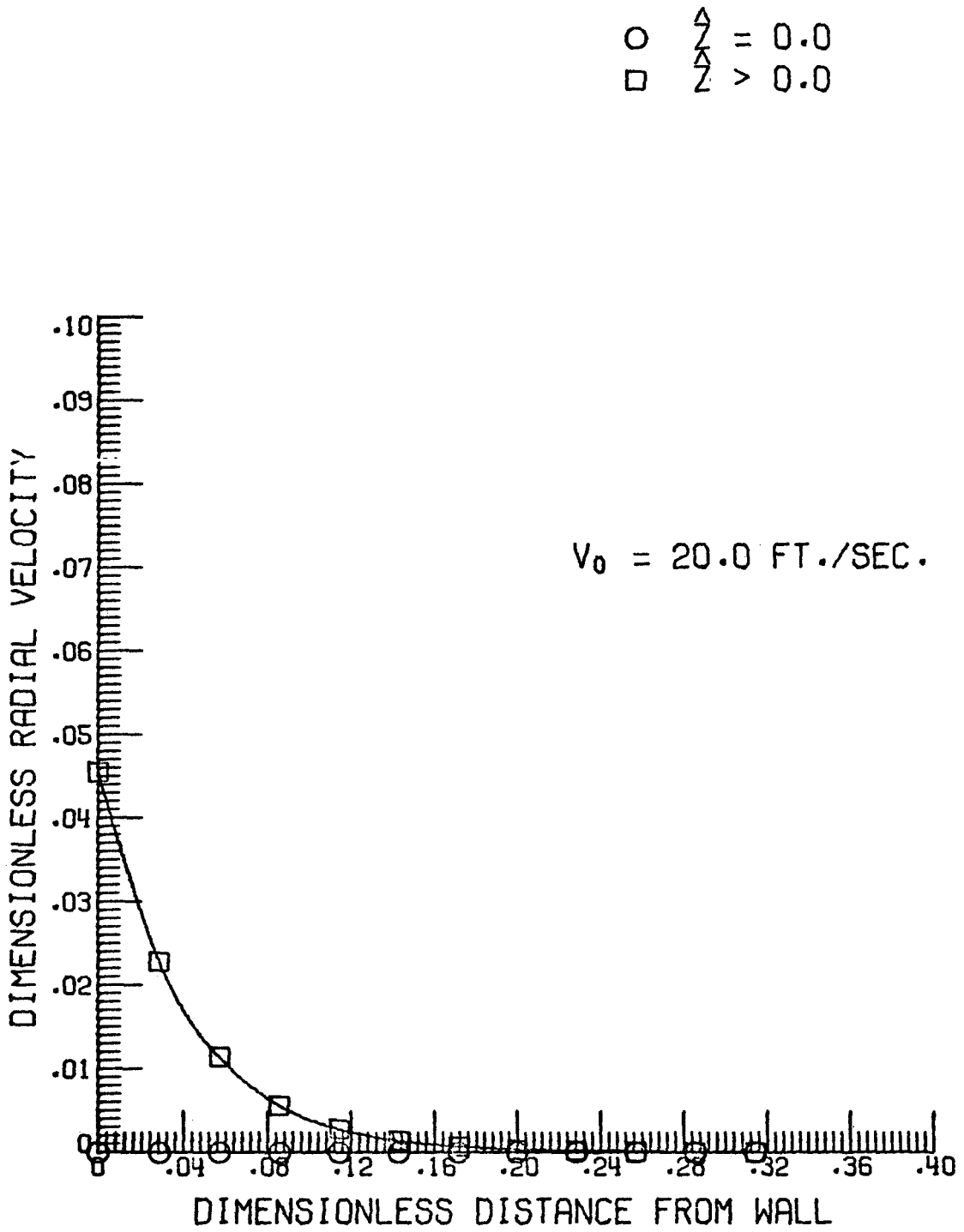


FIGURE (VII-2.5)
INITIAL PROFILE IN GAS PHASE

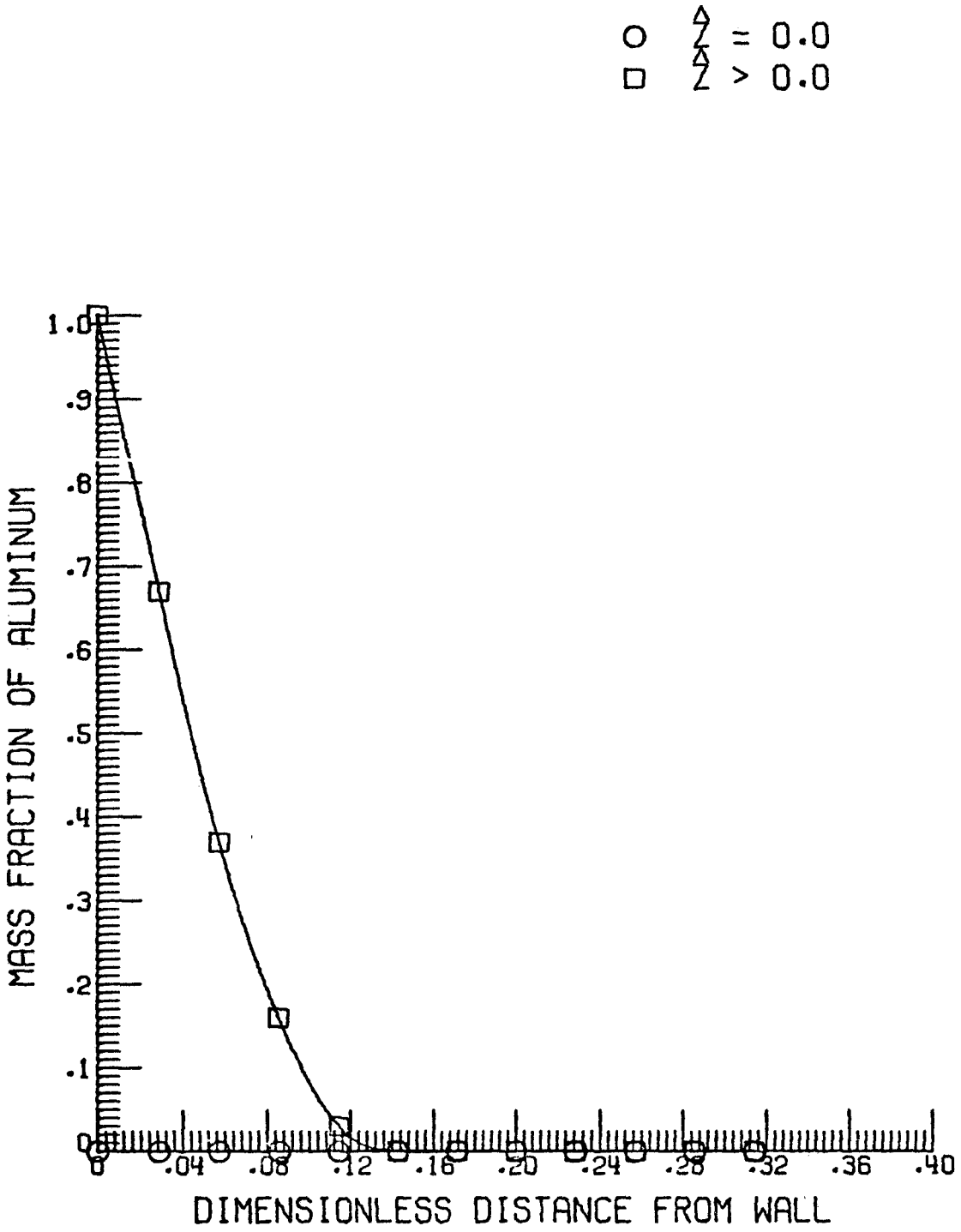


FIGURE (VII-2.6)
INITIAL PROFILE IN GAS PHASE

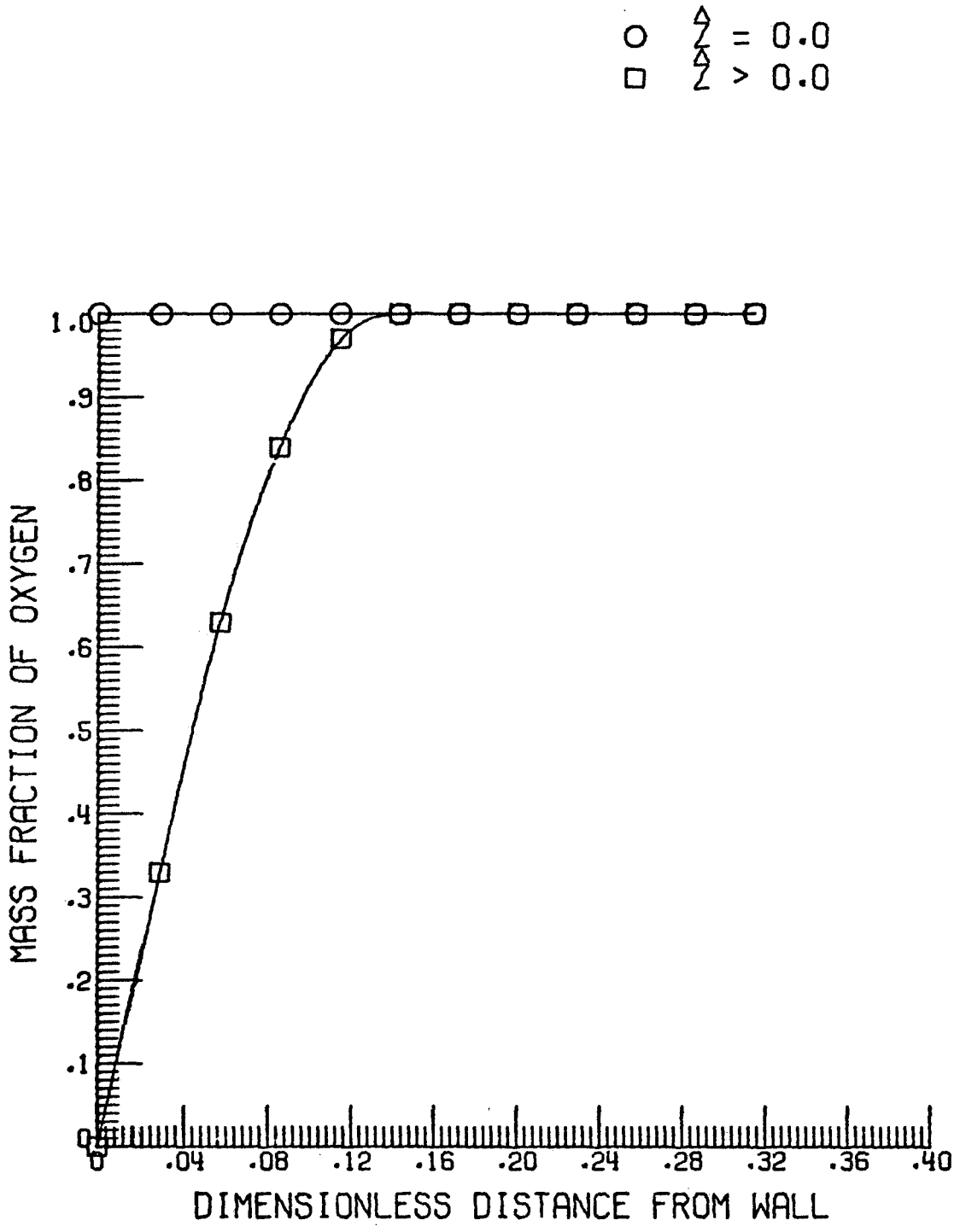


FIGURE (VII-2.7)
INITIAL PROFILE IN GAS PHASE

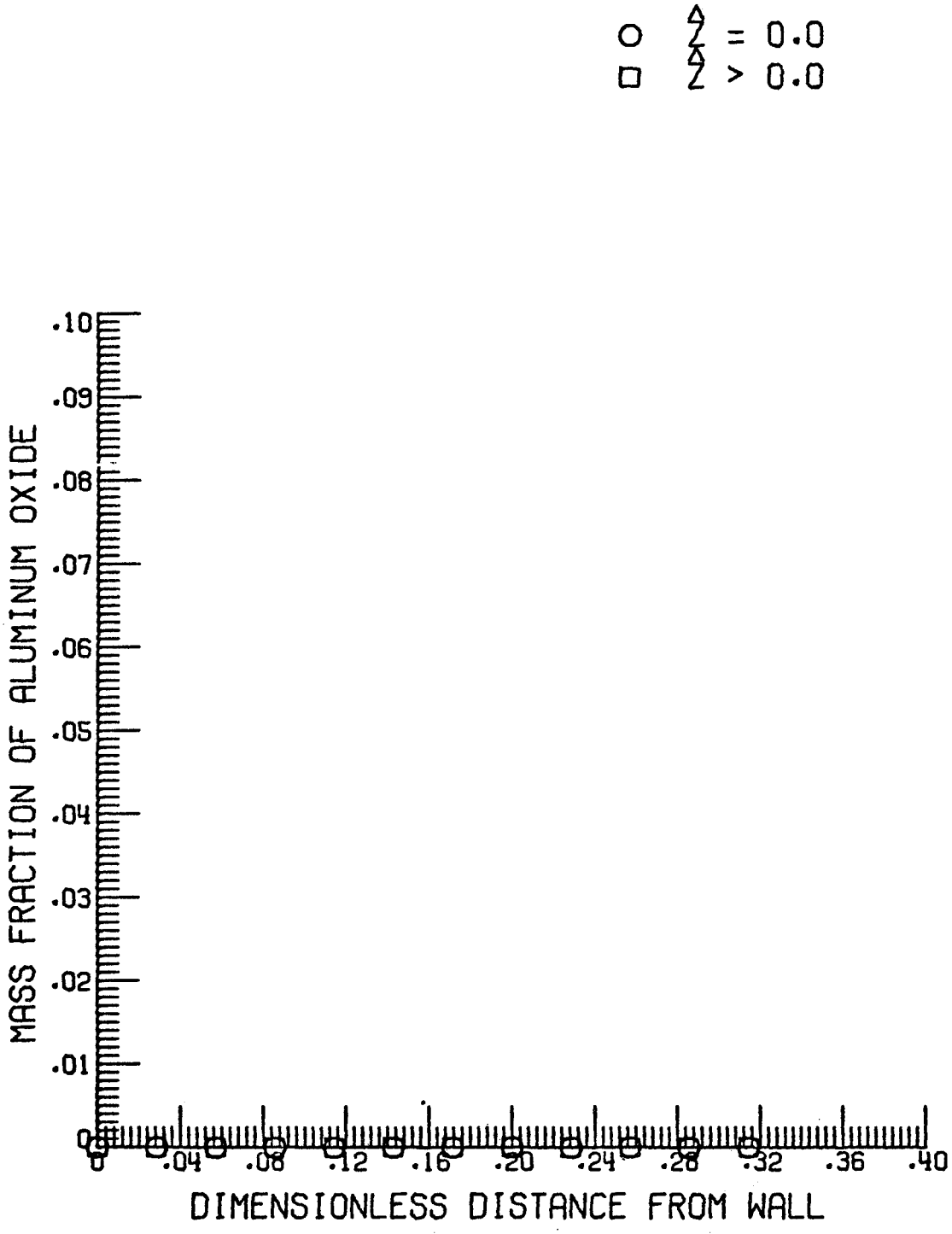
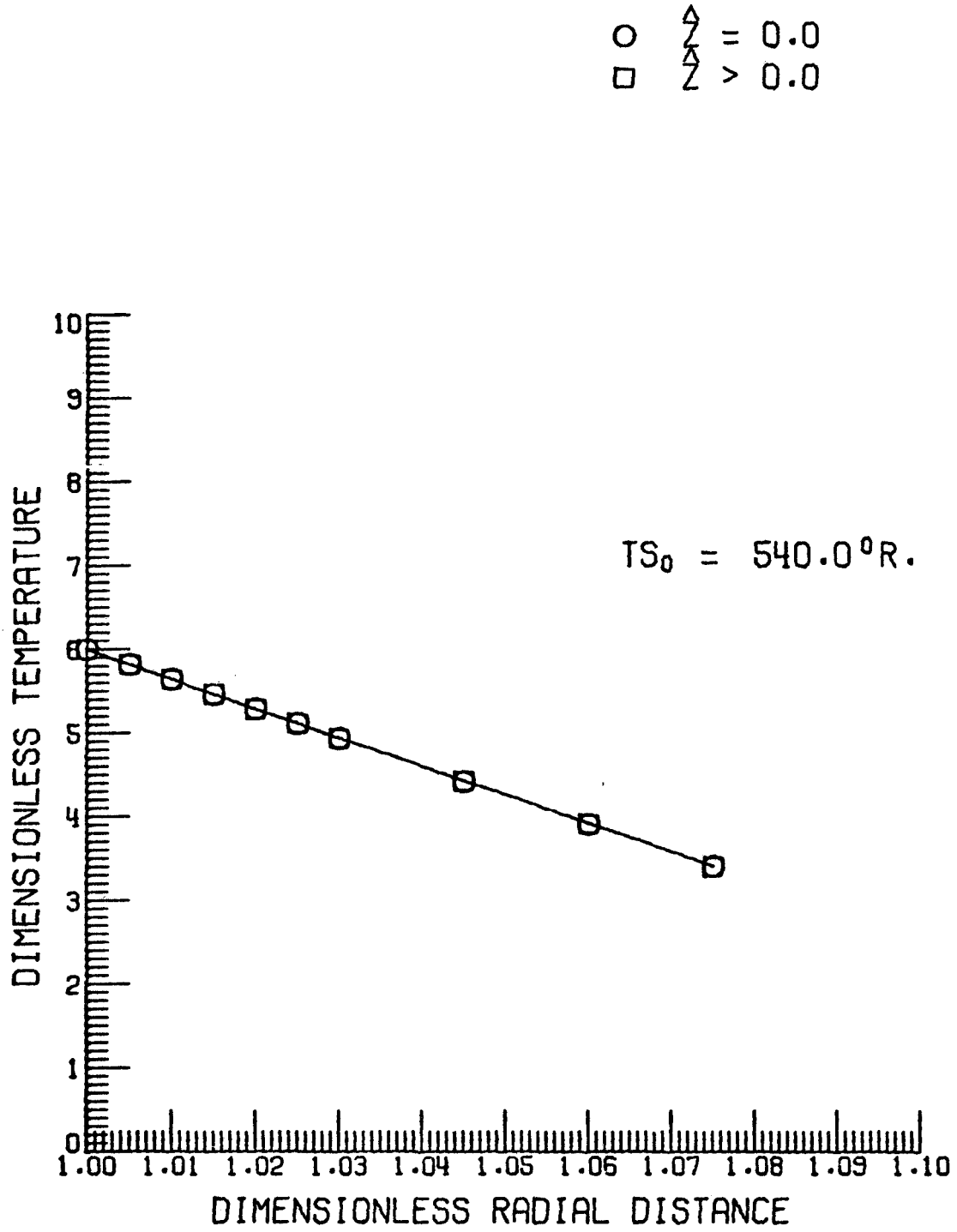


FIGURE (VII-2.8)
INITIAL PROFILE IN SOLID PHASE



The plotted transient data for the gas phase temperature as shown in Figure VII-3.1 - VII-3.3 indicate that the relatively cold gaseous oxygen supply from the inlet actually blows out the initially started flame. This is further demonstrated by the plotted transient data for the mass fraction of Al_2O_3 as shown in Figures VII-4.1 - VII-4.3. Initially, the production of Al_2O_3 in the flame zone at any axial position is spontaneous. The mass fraction of Al_2O_3 diminishes after the required time is allowed for the inlet oxygen supply to reach the particular axial position. The steady-state solutions for the gas phase temperature and the mass fraction of Al, O_2 and Al_2O_3 as shown in Figure VII-5.1 - VII-5.4 indicate that no sustaining gas phase chemical reaction is possible under the prescribed conditions. This points to the fact that the combustion model used is inadequate.

It has been pointed out by Newhall (55), and, Kassoy and Williams (57) that the reaction orders for the fuel and oxidizer are not necessarily the same as the corresponding stoichiometric coefficients for a one-step overall reaction. It appears that the overall reaction orders with respect to the fuel and oxidizer should be found either experimentally or through a detail analysis of the actual reaction mechanism. Since both experimental data and reaction mechanism for the gas phase aluminum-oxygen reaction are not available, arbitrary values were selected for the reaction orders with respect to aluminum and oxygen for the purpose of demonstrating that a flame can be sustained. Hence, if the reaction, $2Al + O_2 \rightarrow 2AlO$, is assumed to be the rate controlling step for the overall reaction, $2Al + 1.5O_2 \rightarrow Al_2O_3$, then,

Figure VII-3.1 - VII-3.3 Transient Gas Phase Temperature Profile at Axial Positions $\hat{Z}$ = 0.12, 0.24 and 0.36

FIGURE (VII-3.1)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .12 .
IN GAS PHASE

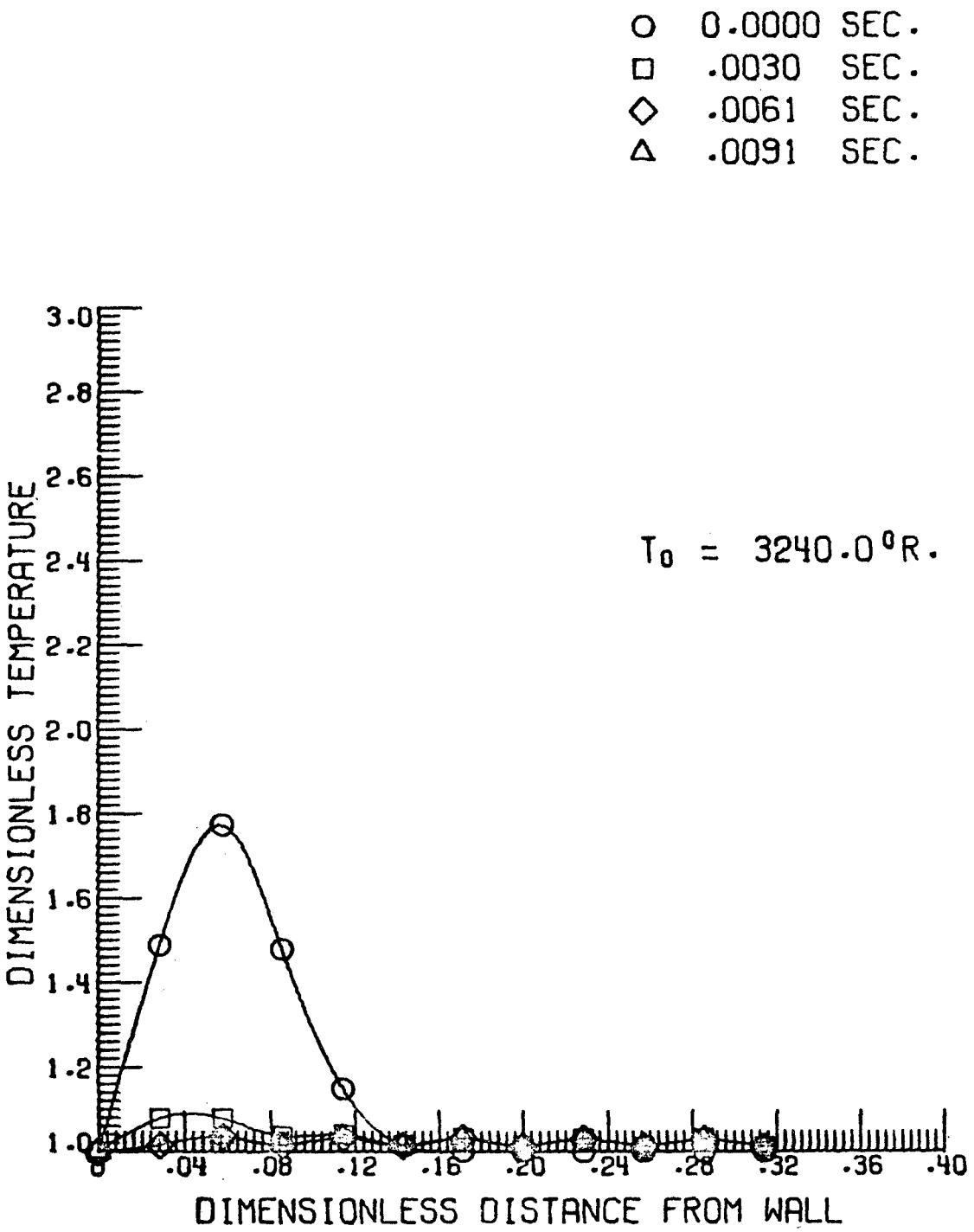


FIGURE (VII-3.2)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .24 .
IN GAS PHASE

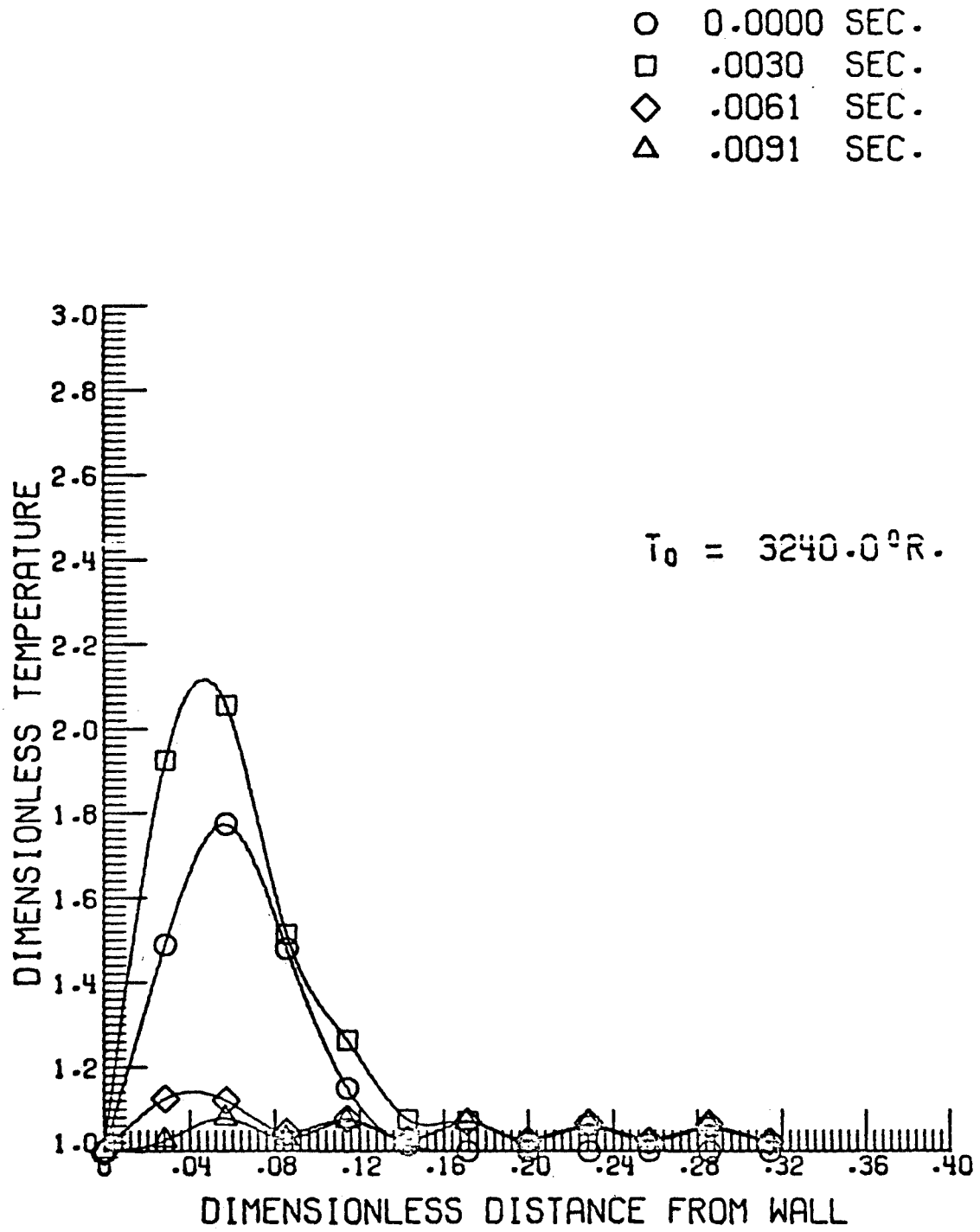


FIGURE (VII-3.3)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .36 .
IN GAS PHASE

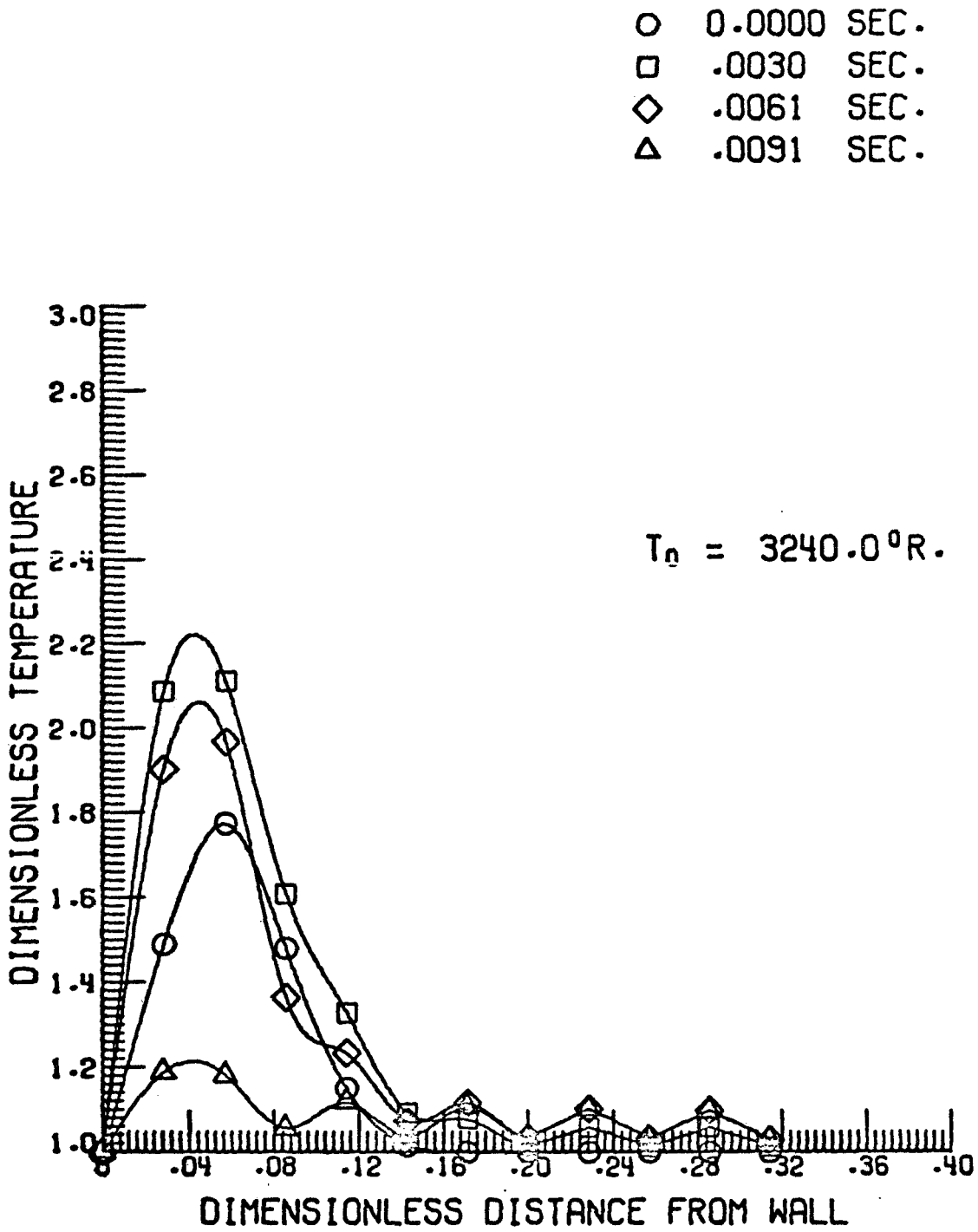


Figure VII-4.1 - VII-4.3 Transient Profile of Al_2O_3 at Axial Position, $\hat{Z}$ = 0.12, 0.24, and 0.36

FIGURE (VII-4.1)
PROFILE AT AXIAL POSITION. $\hat{Z}$ =.12 .
IN GAS PHASE

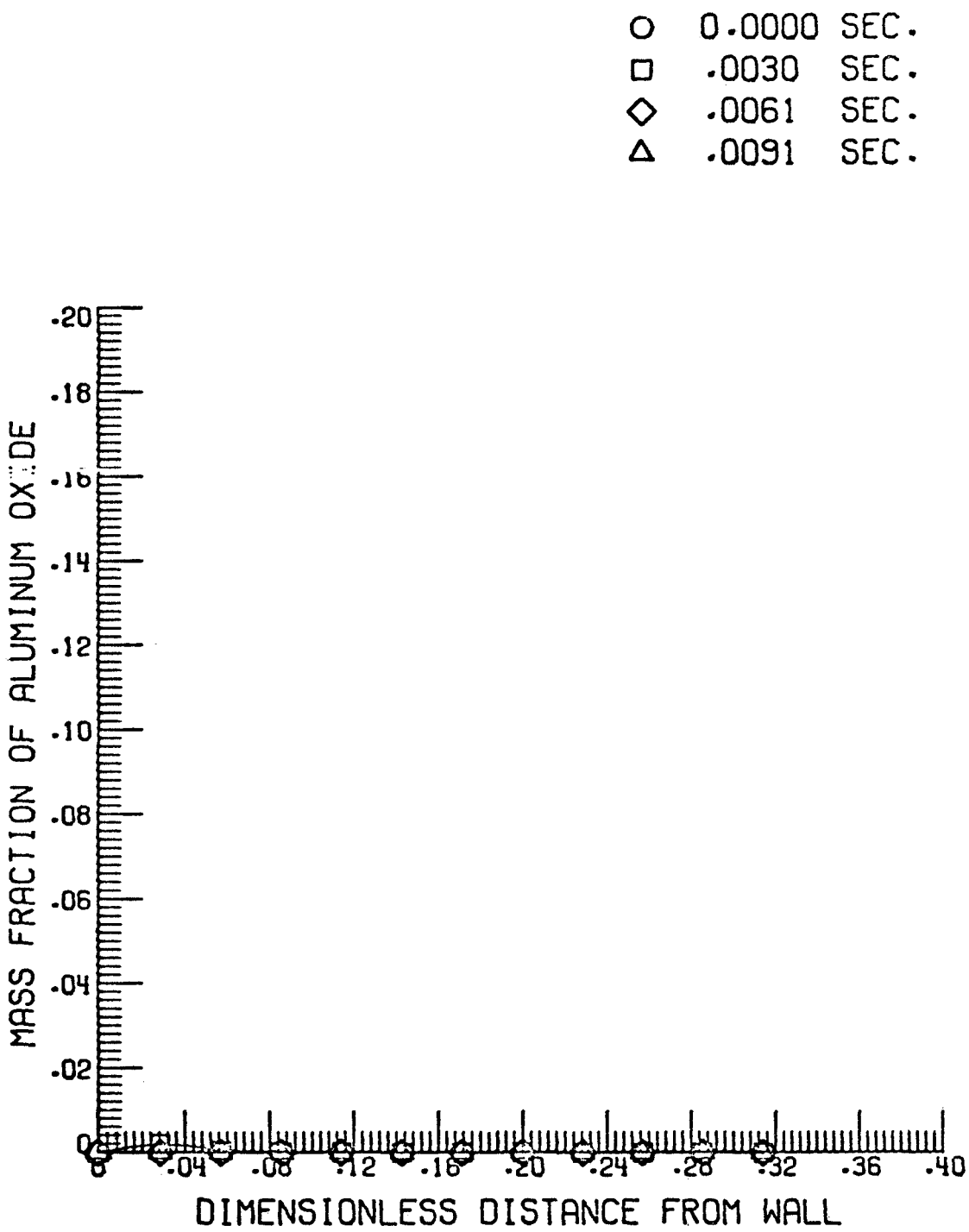


FIGURE (VII-4.2)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .24 .
IN GAS PHASE

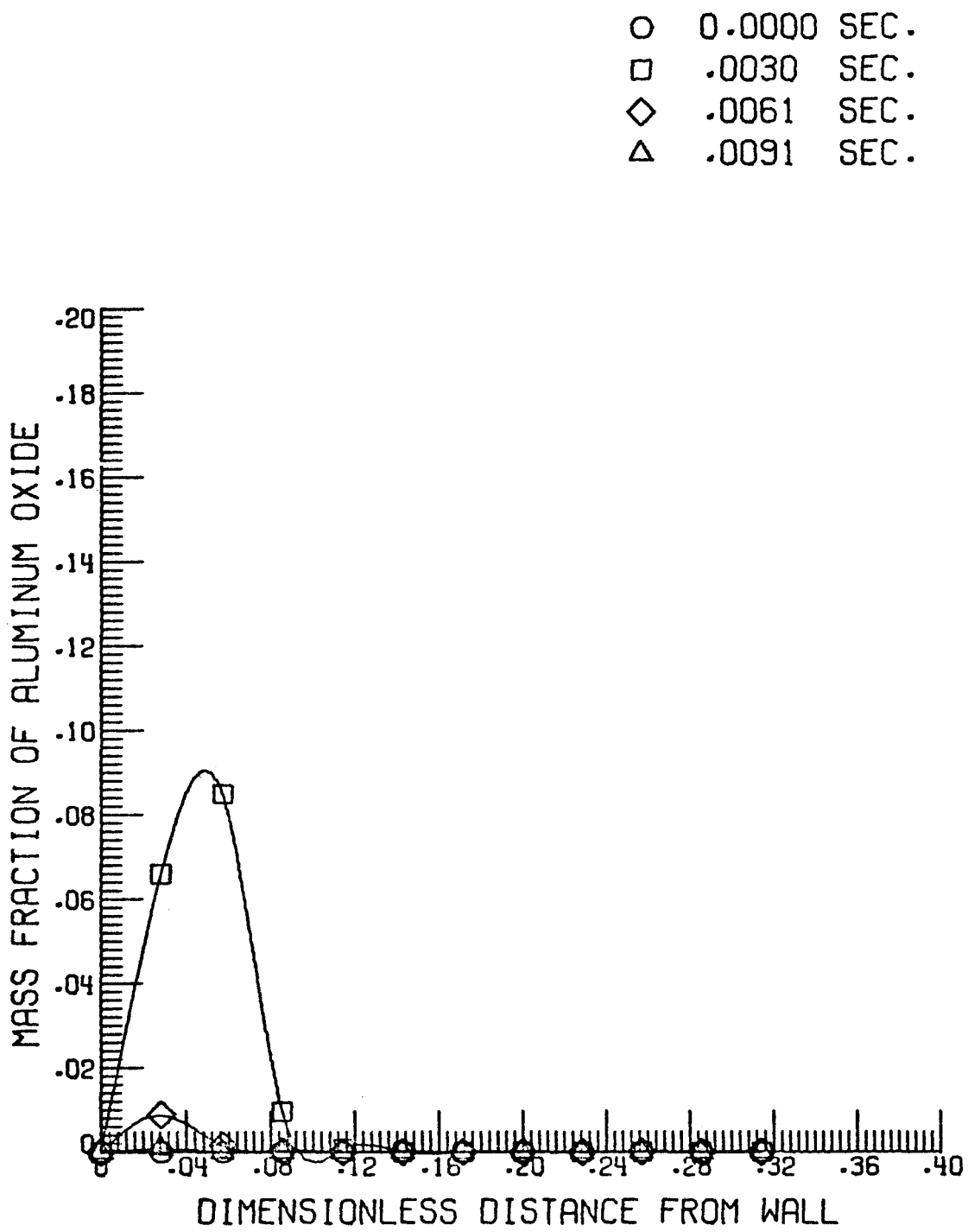


FIGURE (VII-4.3)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .36 .
IN GAS PHASE

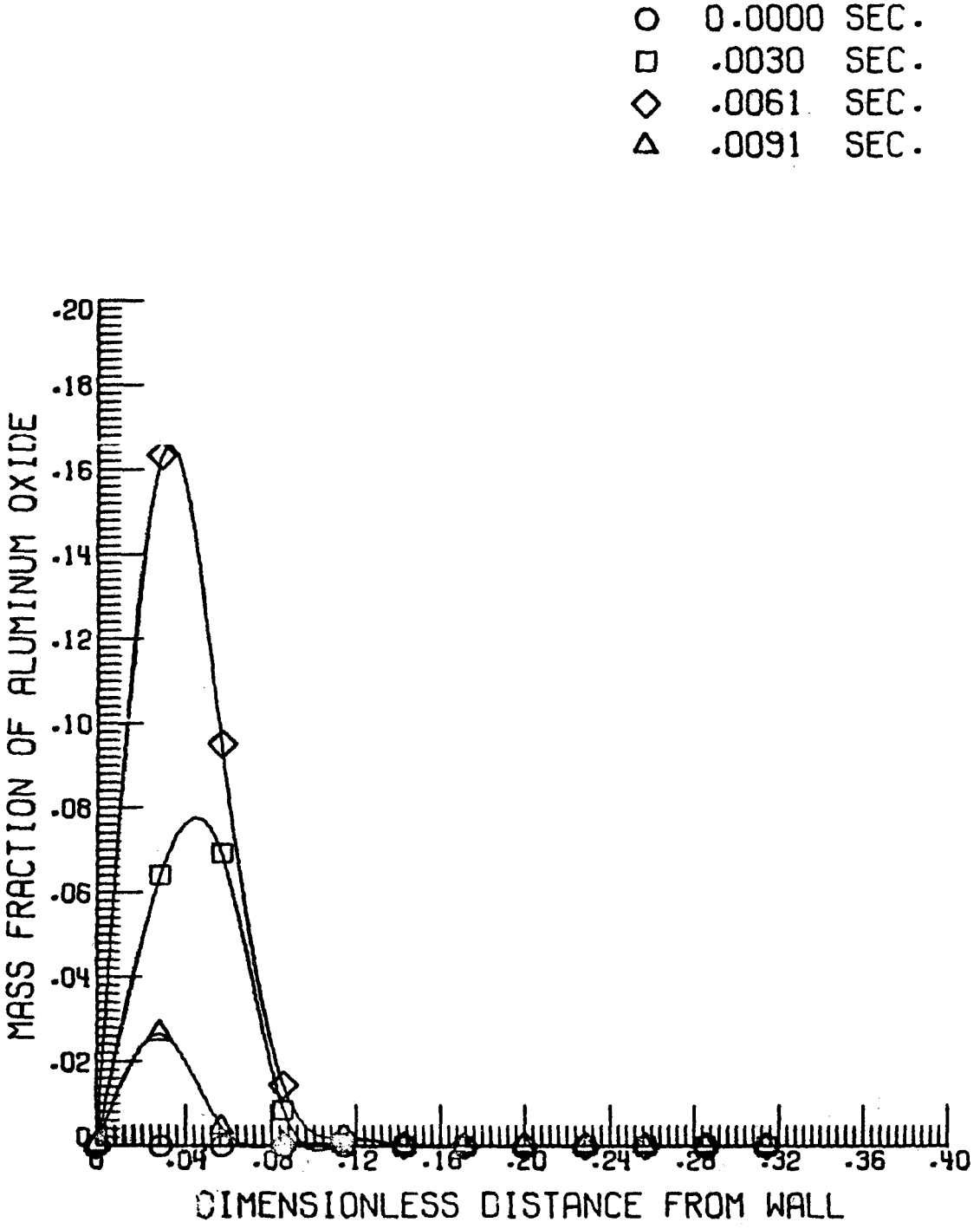


Figure VII-5.1 - VII-5.4 Steady-State Profile for Gas Phase Temperature, Mass Fraction of Aluminum, Oxygen and Aluminum Oxide

FIGURE (VII-5.1)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

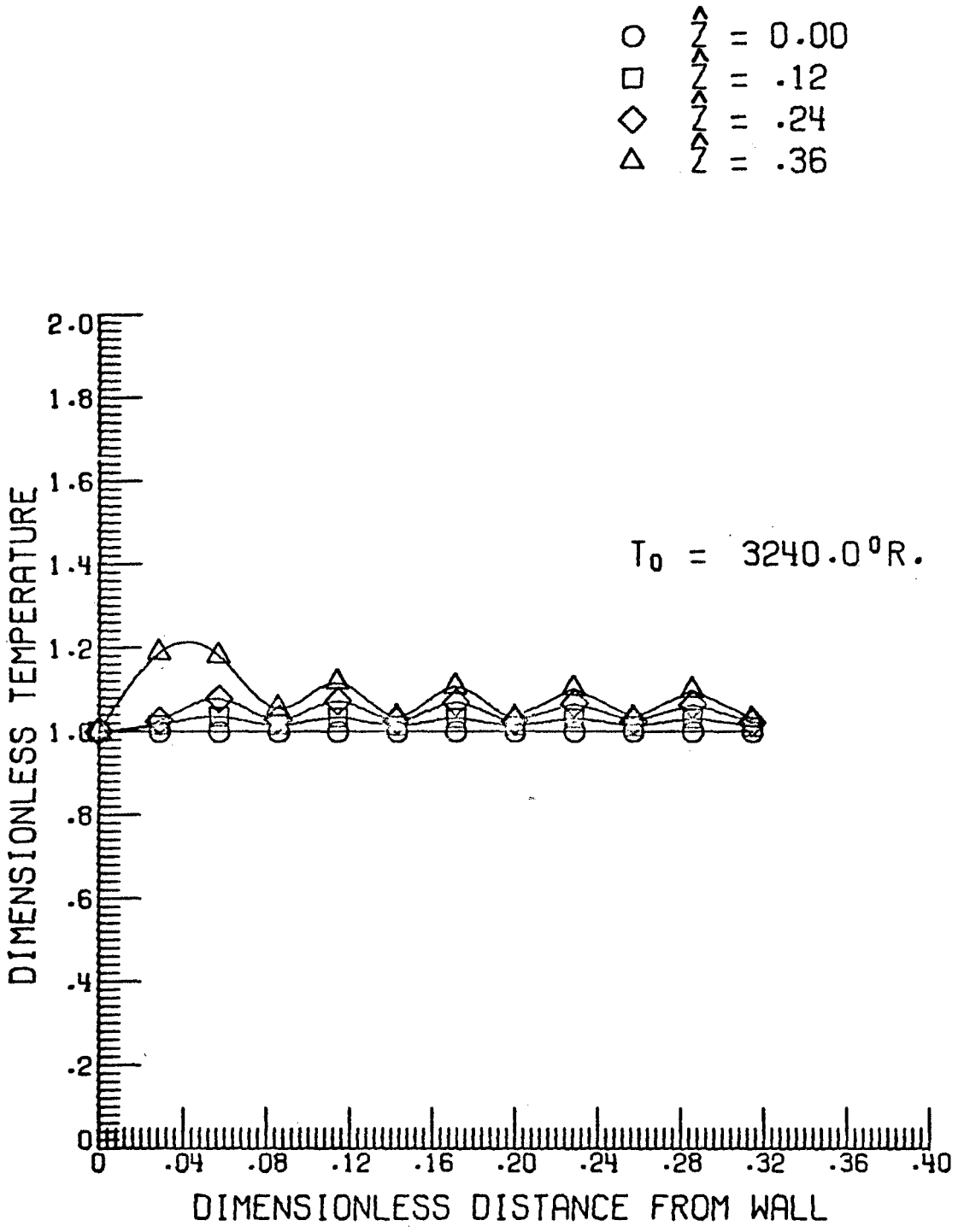


FIGURE (VII-5.2)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

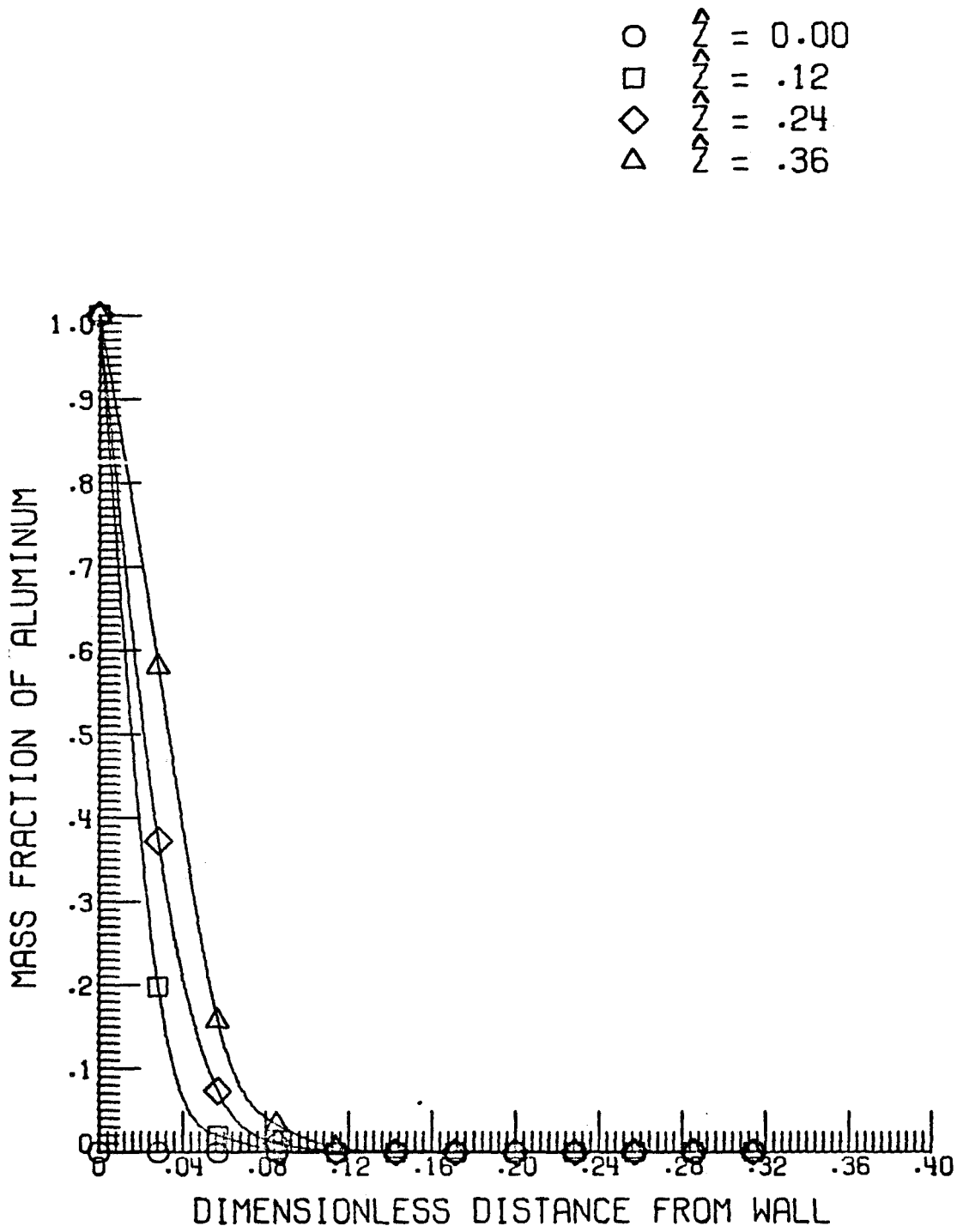


FIGURE (VII-5.3)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

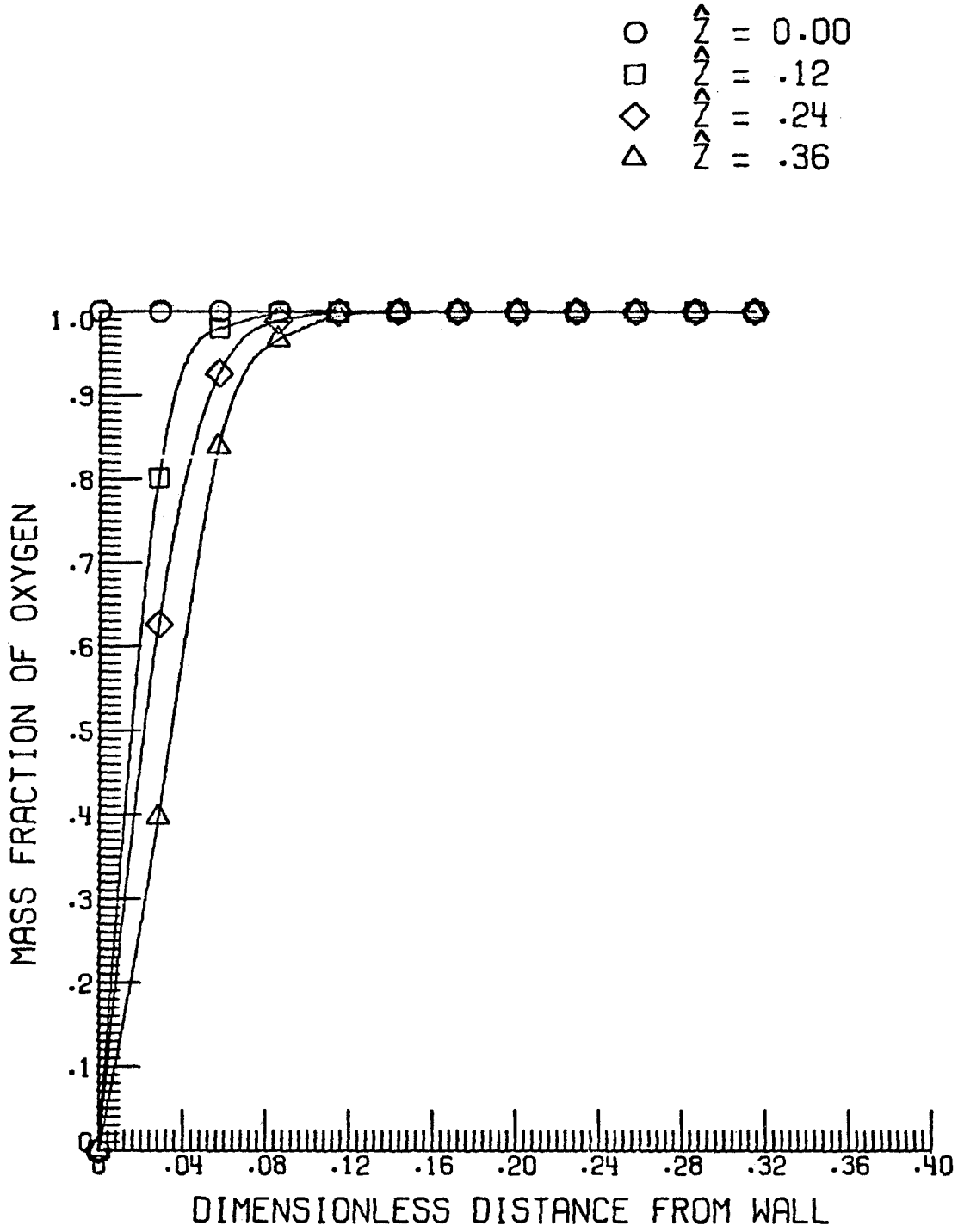
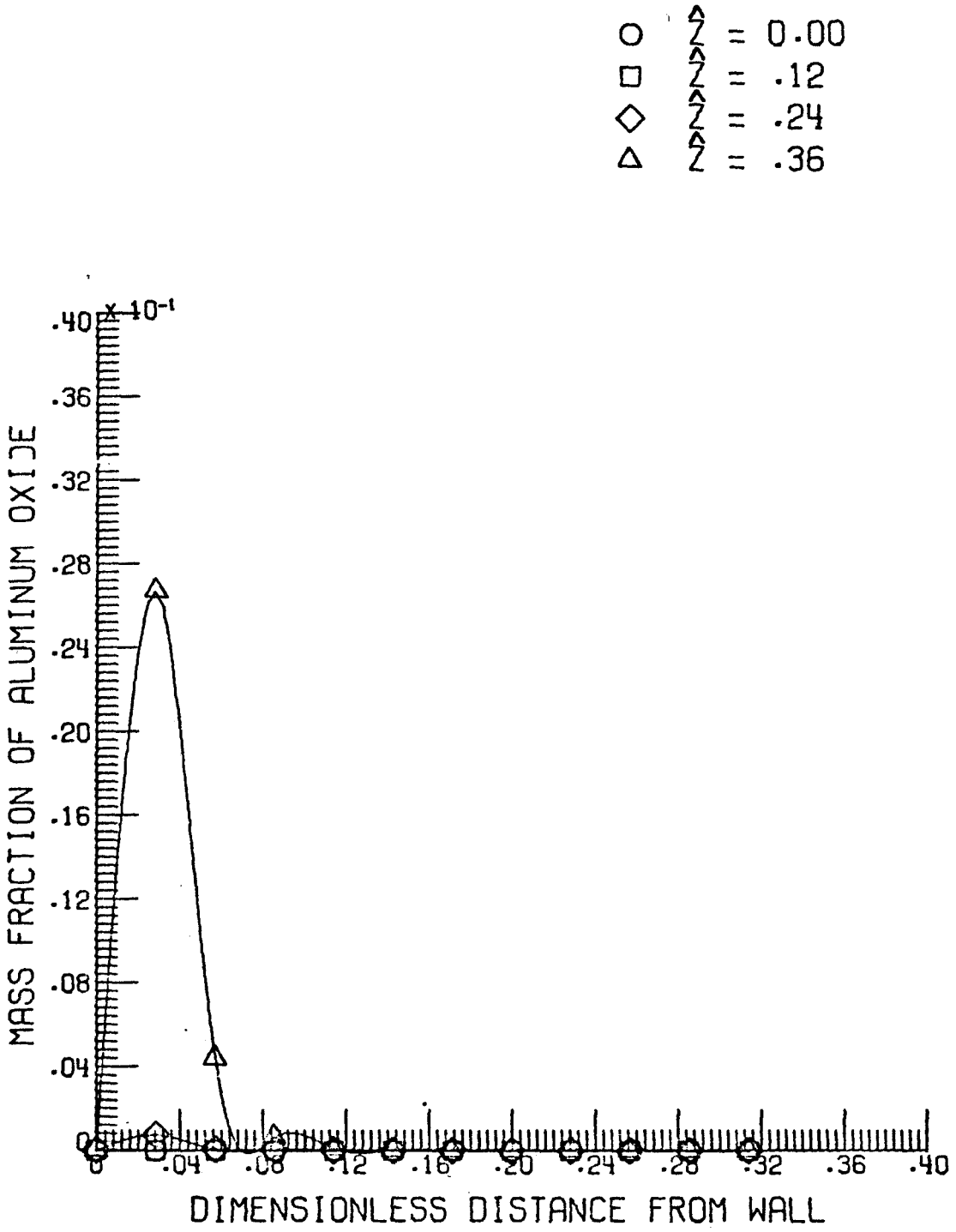


FIGURE (VII-5.4)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE



2.0 and 1.0 in place of 2.0 and 1.5 can be selected as the overall reaction orders with respect to aluminum and oxygen. With $\Delta t \approx 3$ microseconds, numerical calculations were performed for 3000 time steps using the same varying convergence criteria as in the previous case. The calculated results for all the dependent variables at $t \approx 0.003$, 0.006 and 0.009 seconds are included in Appendix D.

In order to get some idea as to the adequacy of the values chosen for the convergence criteria, numerical calculations were performed for the same case with $\Delta t \approx 1.5$ microseconds such that more restricted values of $\zeta = 0.01$ and $\eta = 0.001$ for the convergence criteria could be used. A comparison of the plotted results at $t = 0.003$ second for the two solutions with different convergence criteria shows no significant difference.

With the modified values for the reaction orders, the transient data for the gas phase temperature at axial position, $\hat{z} = 0.12$, 0.24, and 0.36 are plotted as shown in Figures VII-6.1 - VII-6.3. At the start of the combustion process, spontaneous chemical reaction increases the temperature of the initially ignited flame. As the relatively cold oxygen supply from the inlet reaches any of the axial position, a corresponding cooling effect has been observed. Also, the position of the flame as indicated by the peak of the temperature profile is being pushed towards the fuel surface. A sustaining flame can be observed in Figure VII-6.3. A review of the data in Table D-3.2 indicates that the sustaining flame actually starts from axial grid number 9 which is 0.08 ft away from the inlet. From Schlieren and shadowgraph studies by Muzzy (20) and a colored

Figure VII-6.1 - VII-6.3 Transient Gas Phase Temperature Profile at Axial Position, $\hat{Z}$ = 0.12, 0.24 and 0.36, with the Modified Values for the Reaction Orders.

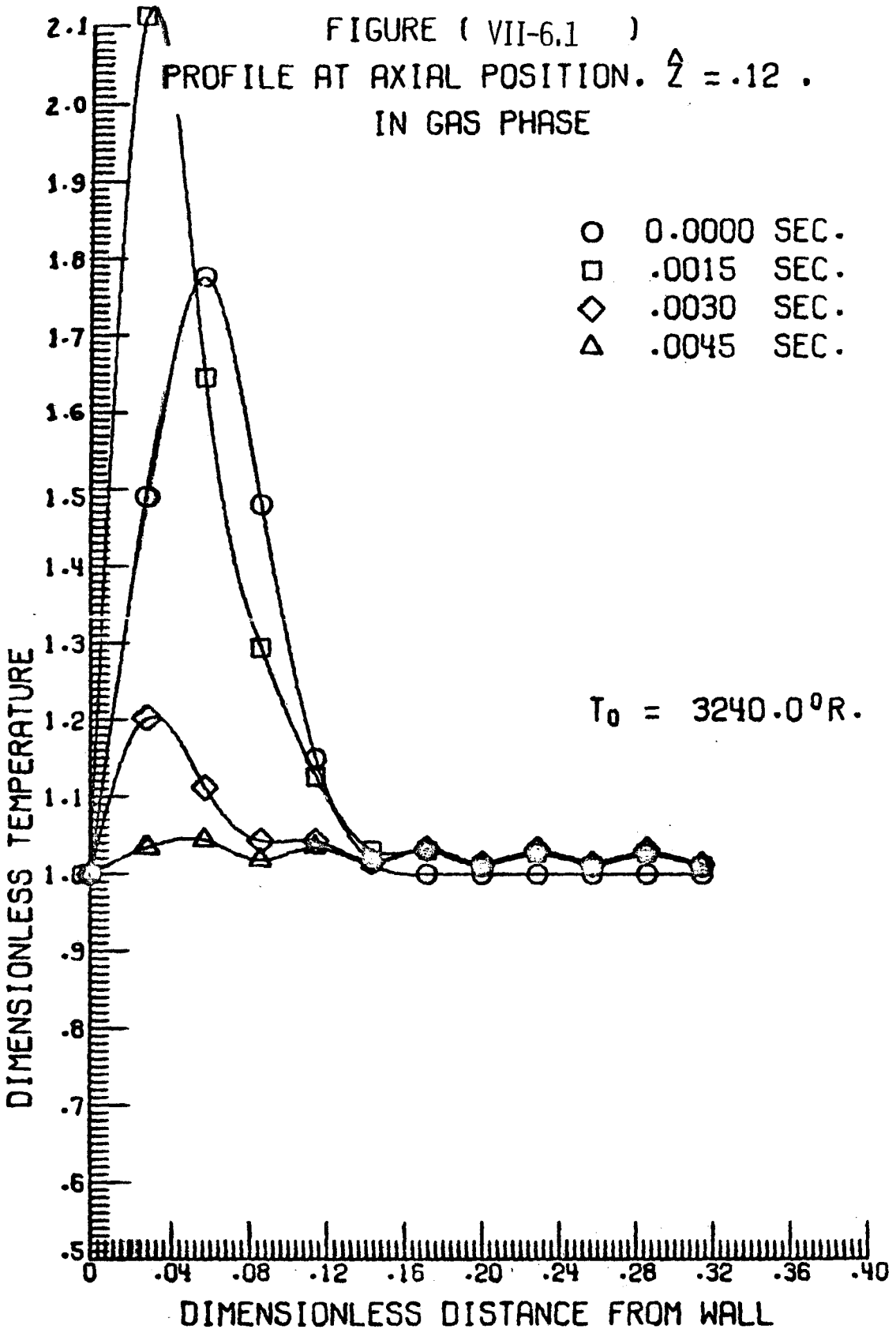


FIGURE (VII-6.1)
PROFILE AT AXIAL POSITION. Ẑ = .12 .
IN GAS PHASE
0.0000 SEC.
.0015 SEC.
.0030 SEC.
.0045 SEC.
T0 = 3240.0 0R.
DIMENSIONLESS TEMPERATURE
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
.9
.8
.7
.6
.5
0
.04
.08
.12
.16
.20
.24
.28
.32
.36
.40
DIMENSIONLESS DISTANCE FROM WALL

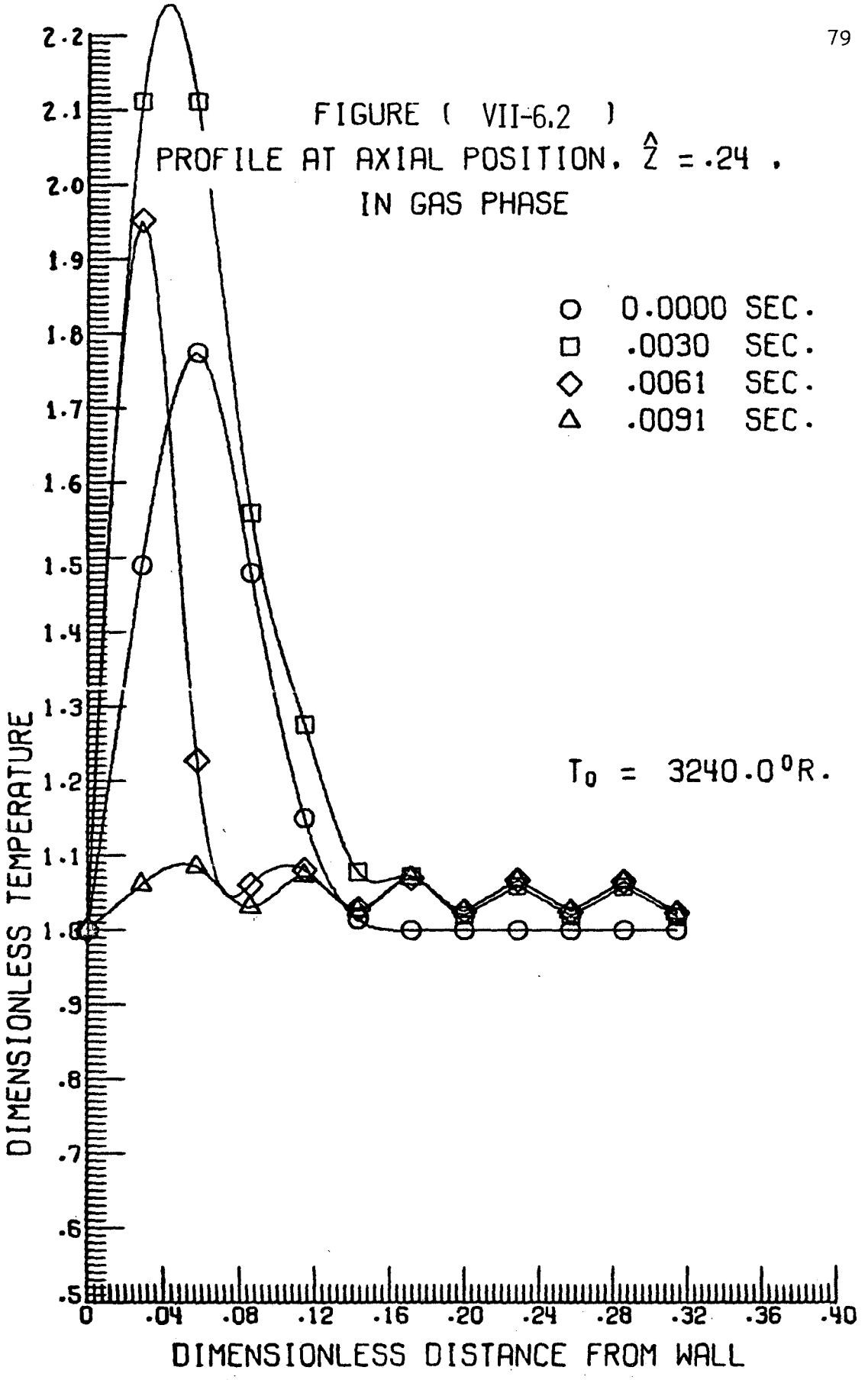
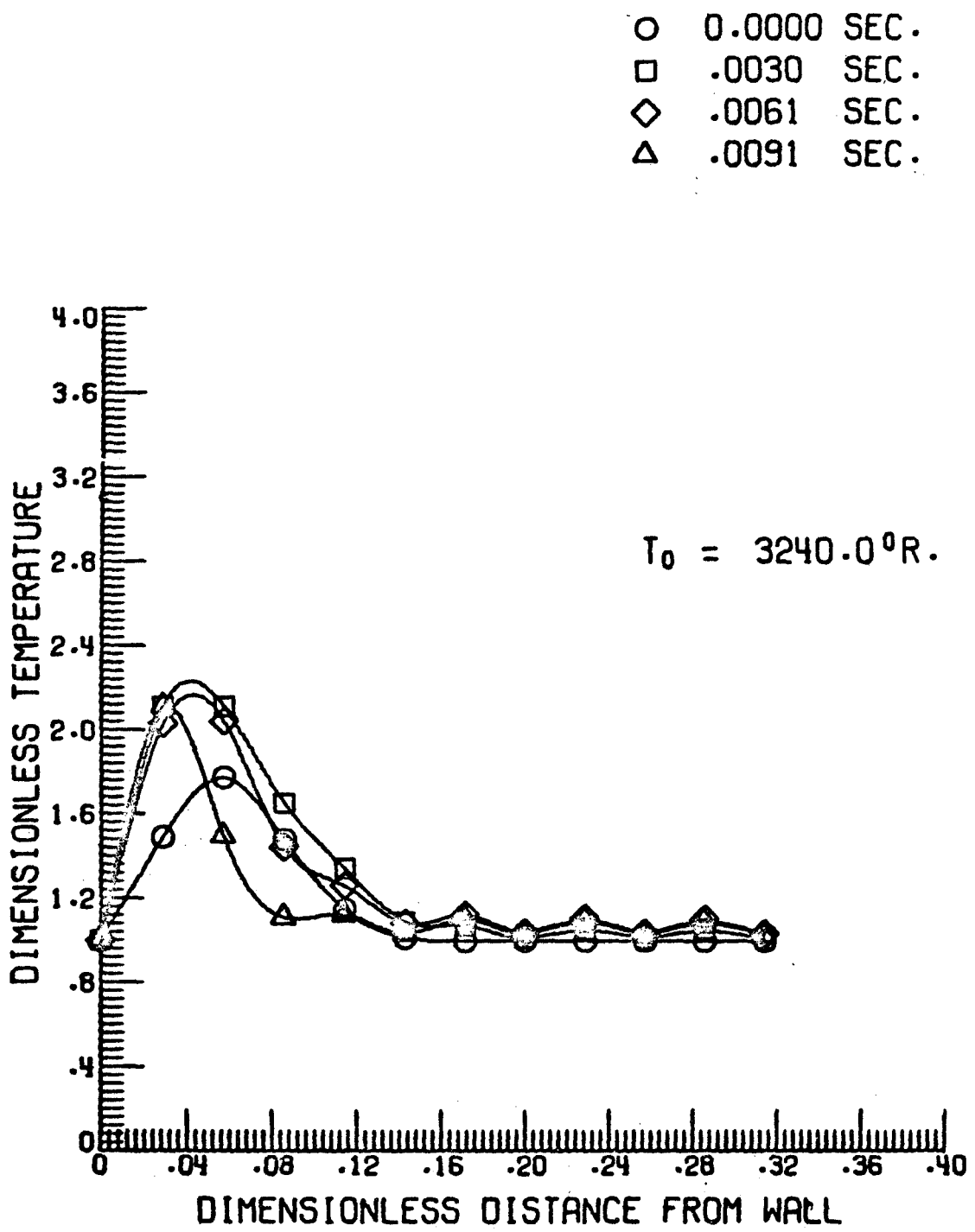


FIGURE (VII-6.2)
PROFILE AT AXIAL POSITION, $\hat{Z}$ = .24 ,
IN GAS PHASE
0.0000 SEC.
.0030 SEC.
.0061 SEC.
.0091 SEC.
T_0 = 3240.0 °R.
DIMENSIONLESS TEMPERATURE
DIMENSIONLESS DISTANCE FROM WALL
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
.9
.8
.7
.6
.5
0
.04
.08
.12
.16
.20
.24
.28
.32
.36
.40

FIGURE (VII-6.3)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .36 .
IN GAS PHASE



movie produced by ONERA (42) on experimental hybrid rocket systems, it has been demonstrated that the distance of the flame position from the fuel surface is zero at the inlet and increases in the downstream axial direction as shown in Figure VII.7. If $\Delta\hat{r}$ is the dimensionless radial grid spacing used, the finite difference method can only approximate a sustaining flame solution a distance approximately equal to $\hat{z}_c$ downstream of the inlet. Apparently, with the coarse grid spacing used in the current solution, this distance is roughly equal to 0.08 ft.

The corresponding transient variation of the mass fraction of Al_2O_3 has been plotted in Figure VII-8.1 - VII-8.3. The production of Al_2O_3 is concentrated in the reaction zone as expected. The transient variation of the mass fraction of Al_2O_3 is fully in accord with the transient temperature variation. The mass fraction of Al_2O_3 decreases back to zero where a sustaining flame solution is not possible and increases continuously where a flame is sustained.

The transient effect on the axial velocity profile due to mass addition and combustion are demonstrated in Figure VII-9.1- VII-9.3. The effect of mass addition and combustion tends to decrease the magnitude of the axial velocity gradient at the fuel surface. This is in good qualitative agreement with the findings of Jones and Isaacson (46) in their experimental work.

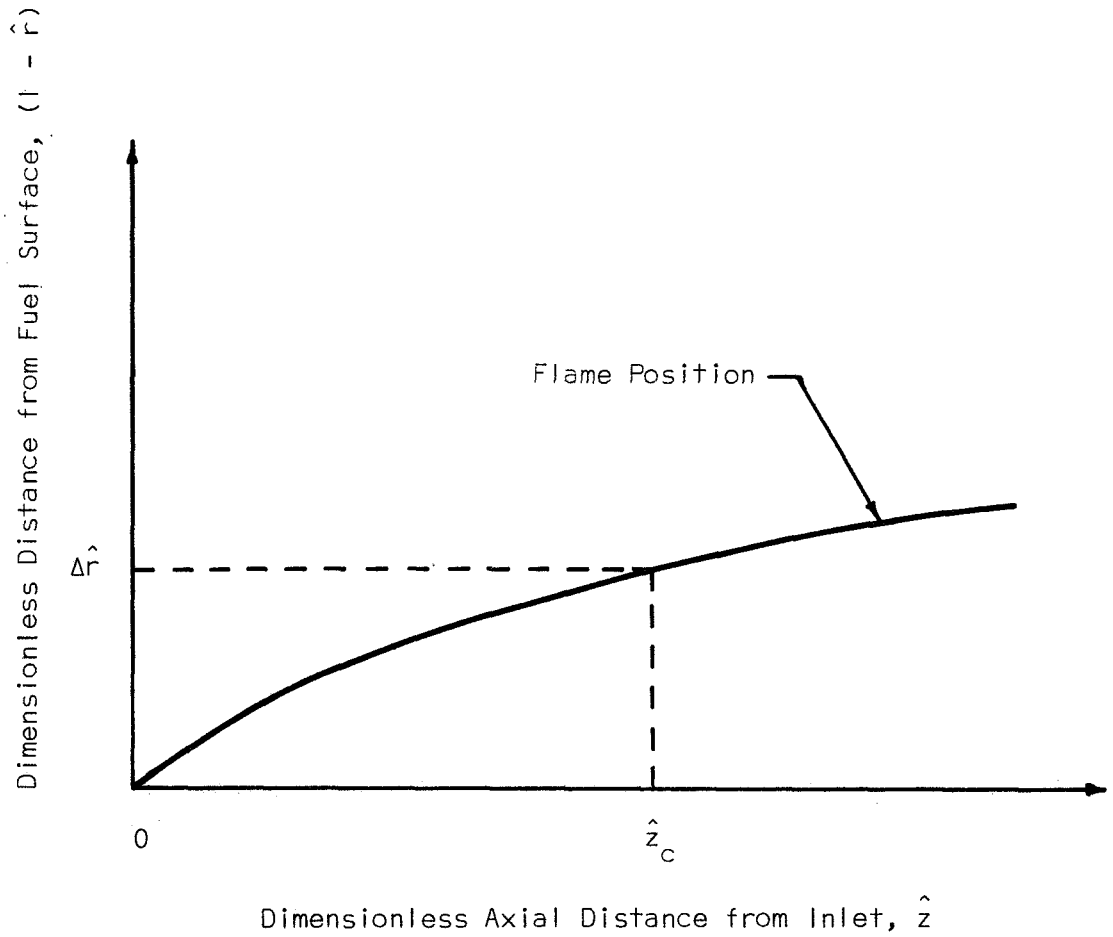


Figure VII.7 Steady-State Flame Position in Hybrid Rocket Combustion Chamber

Figure VII-8.1 - VII-8.3 Transient Profile of Al_2O_3 at Axial Position, $\hat{Z}$ = 0.12, 0.24, and 0.36, with the Modified Values for the Reaction Orders

FIGURE (VII-8.1)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .12 .
IN GAS PHASE

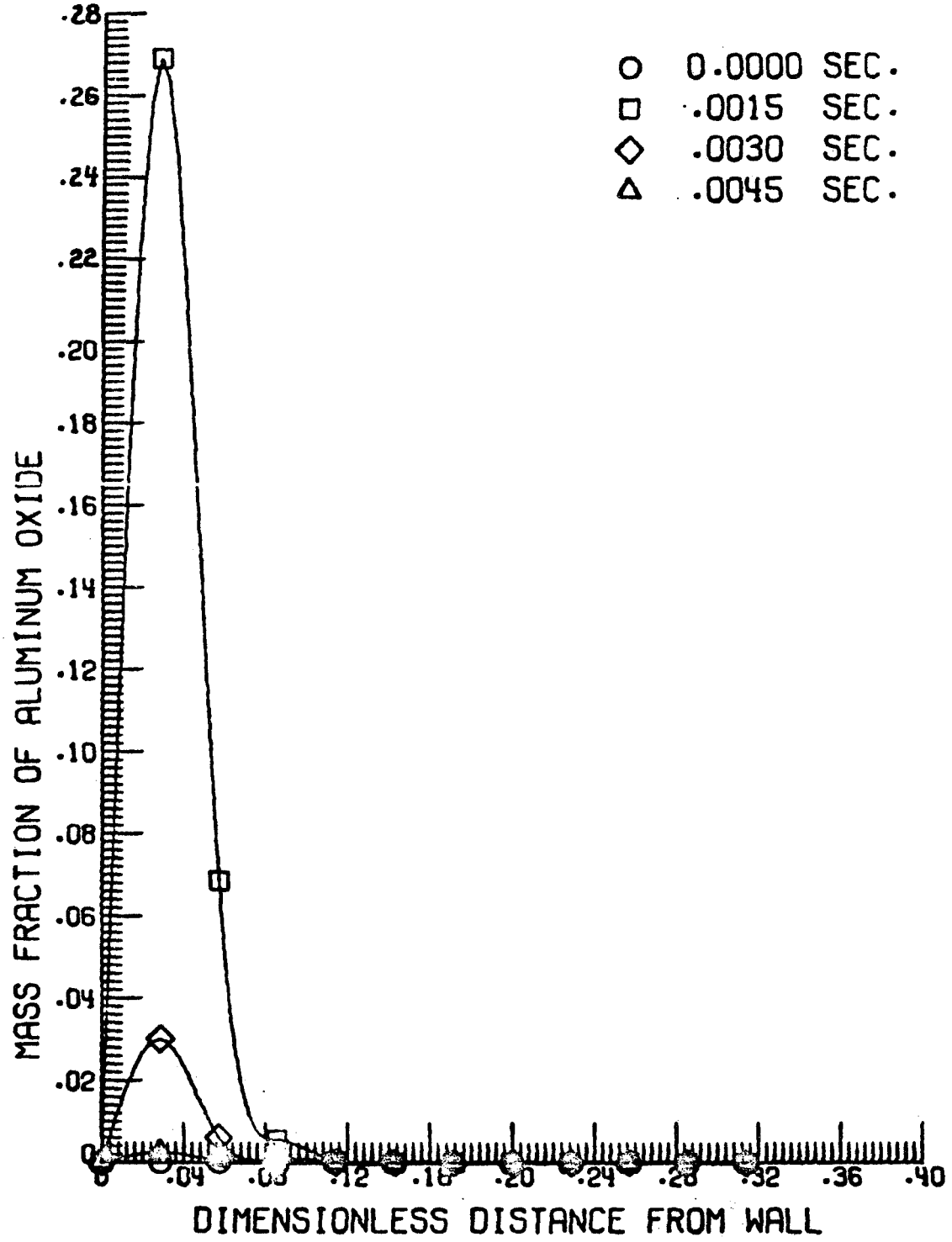


FIGURE (VII-8.2)
PROFILE AT AXIAL POSITION, $\hat{Z}$ = .24 .
IN GAS PHASE

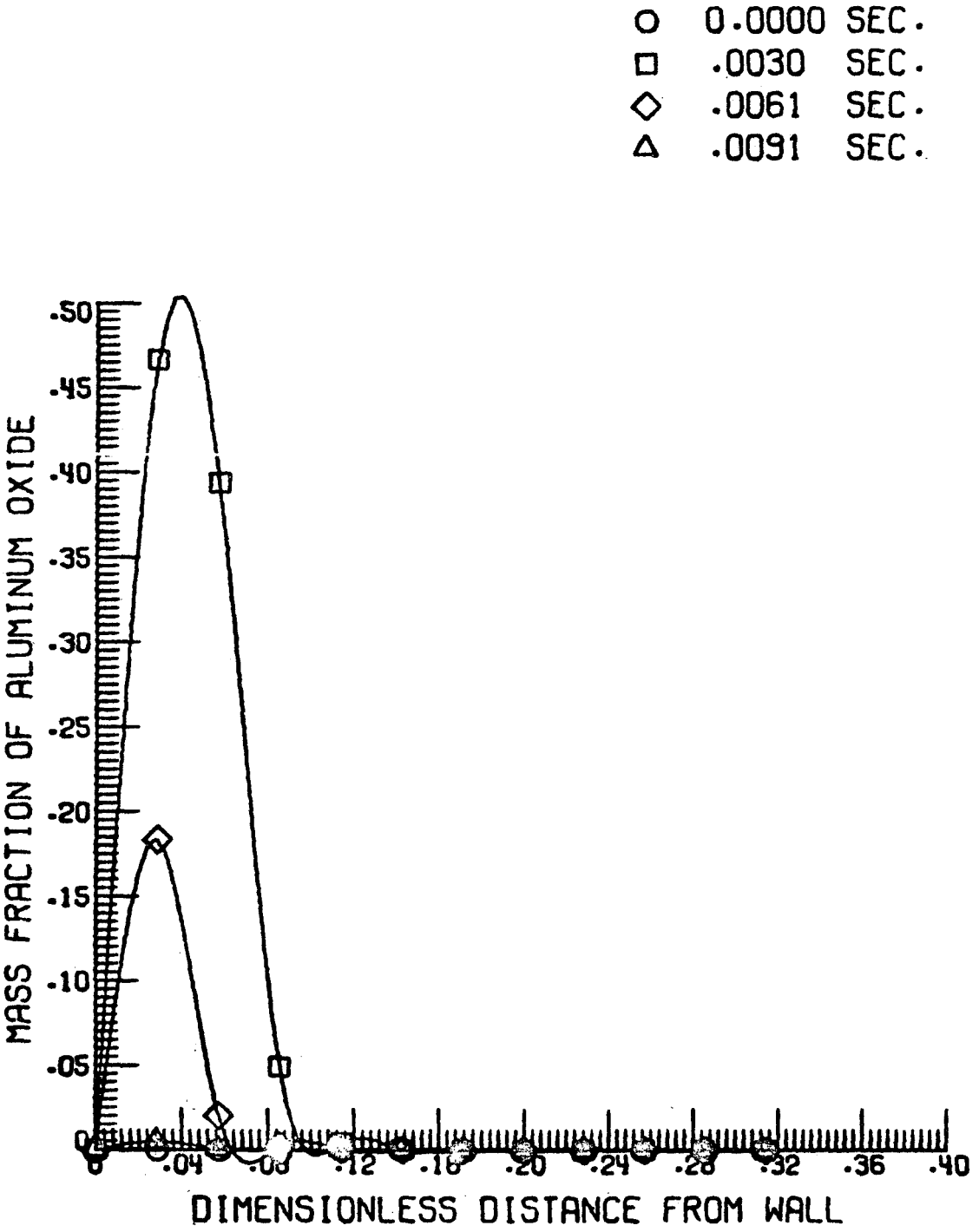


FIGURE (VII-8.3)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .36 .
IN GAS PHASE

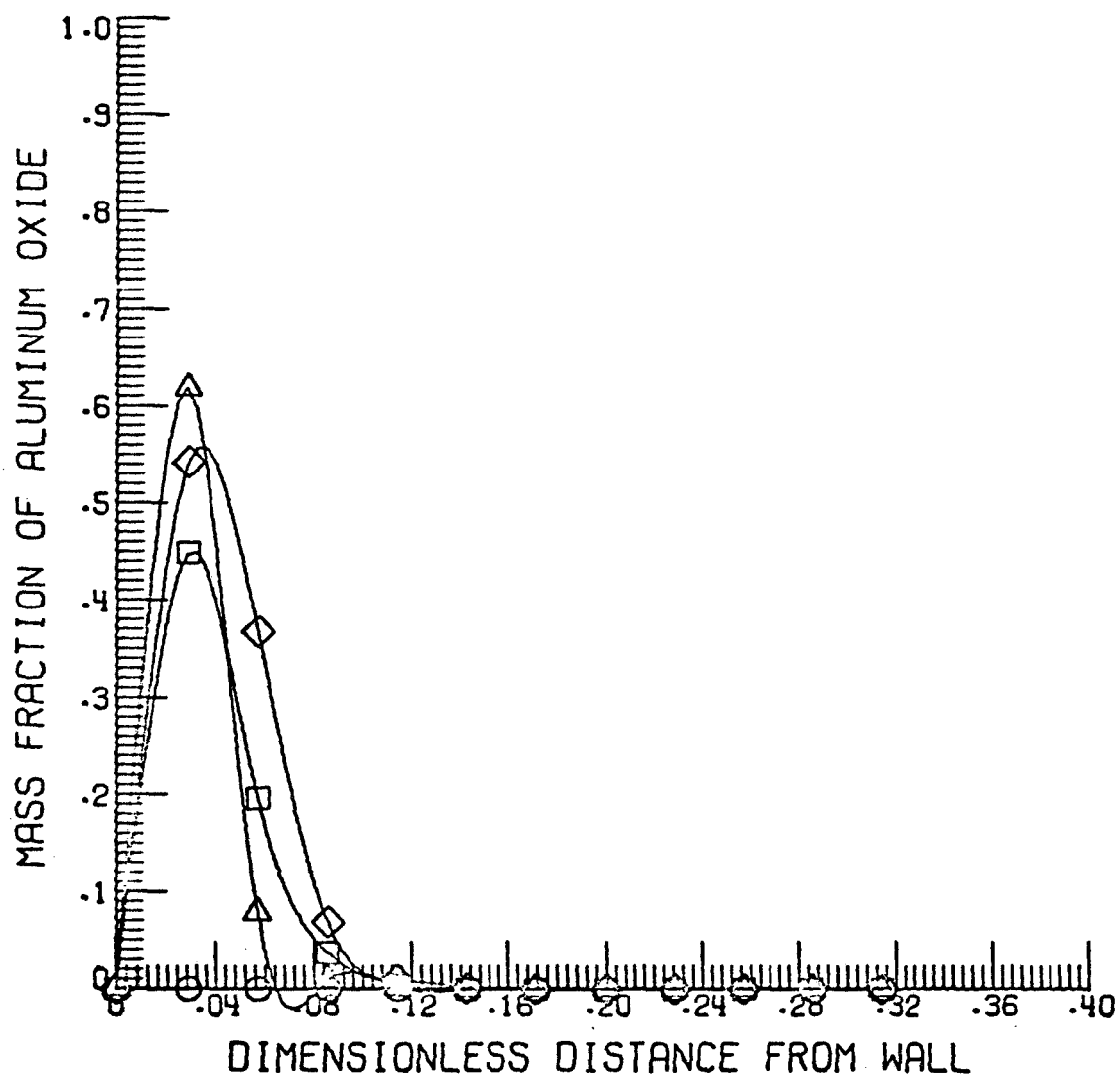


Figure VII-9.1 - VII-9.3 Transient Profile of Axial Velocity Component at Axial Position, $\hat{Z}$ = 0.12, 0.24 and 0.36, with the Modified Values for the Reaction Orders

FIGURE (VII-9.1)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .12 .
IN GAS PHASE

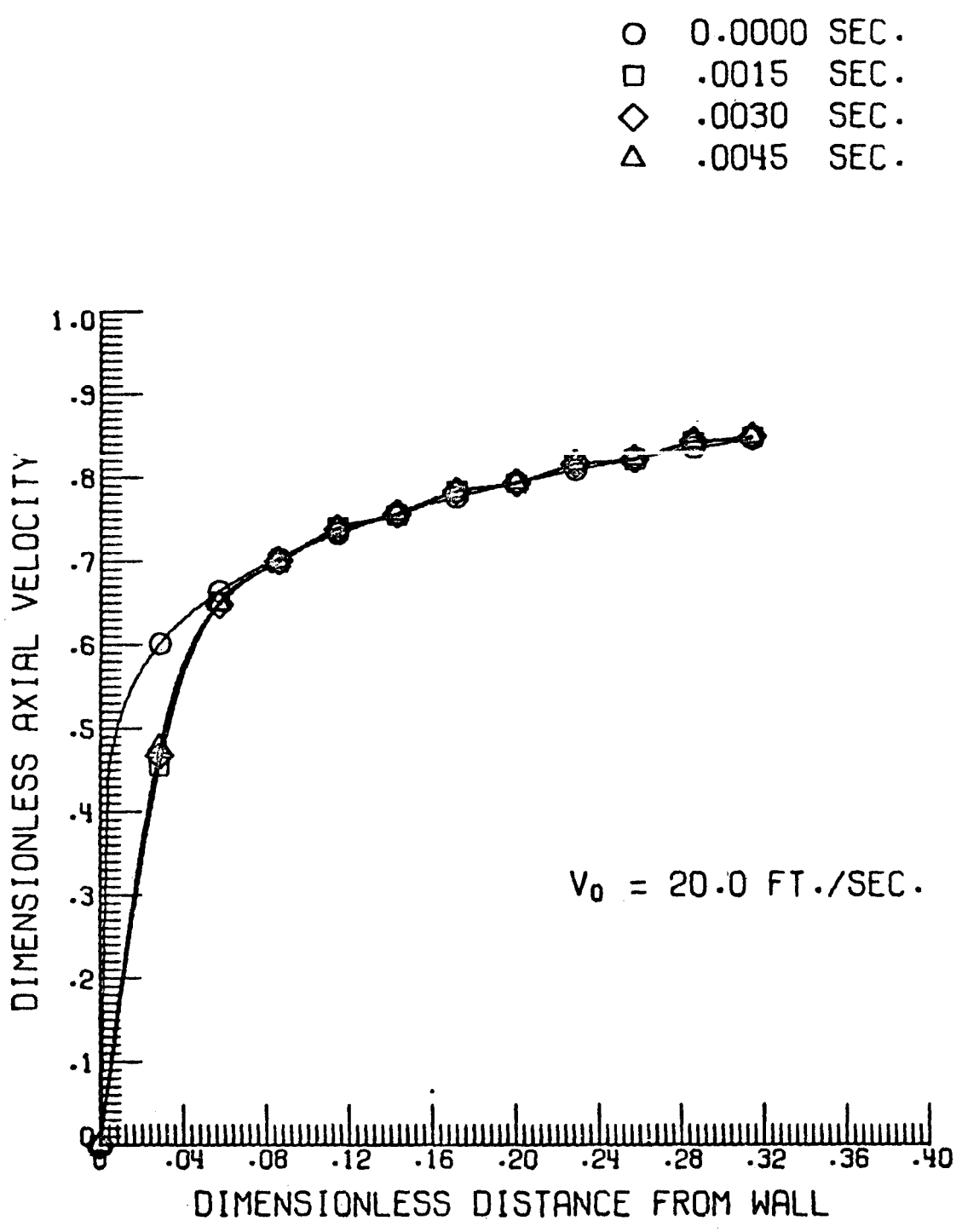


FIGURE (VII-9.2)
PROFILE AT AXIAL POSITION. $\hat{z}$ = .24 .
IN GAS PHASE

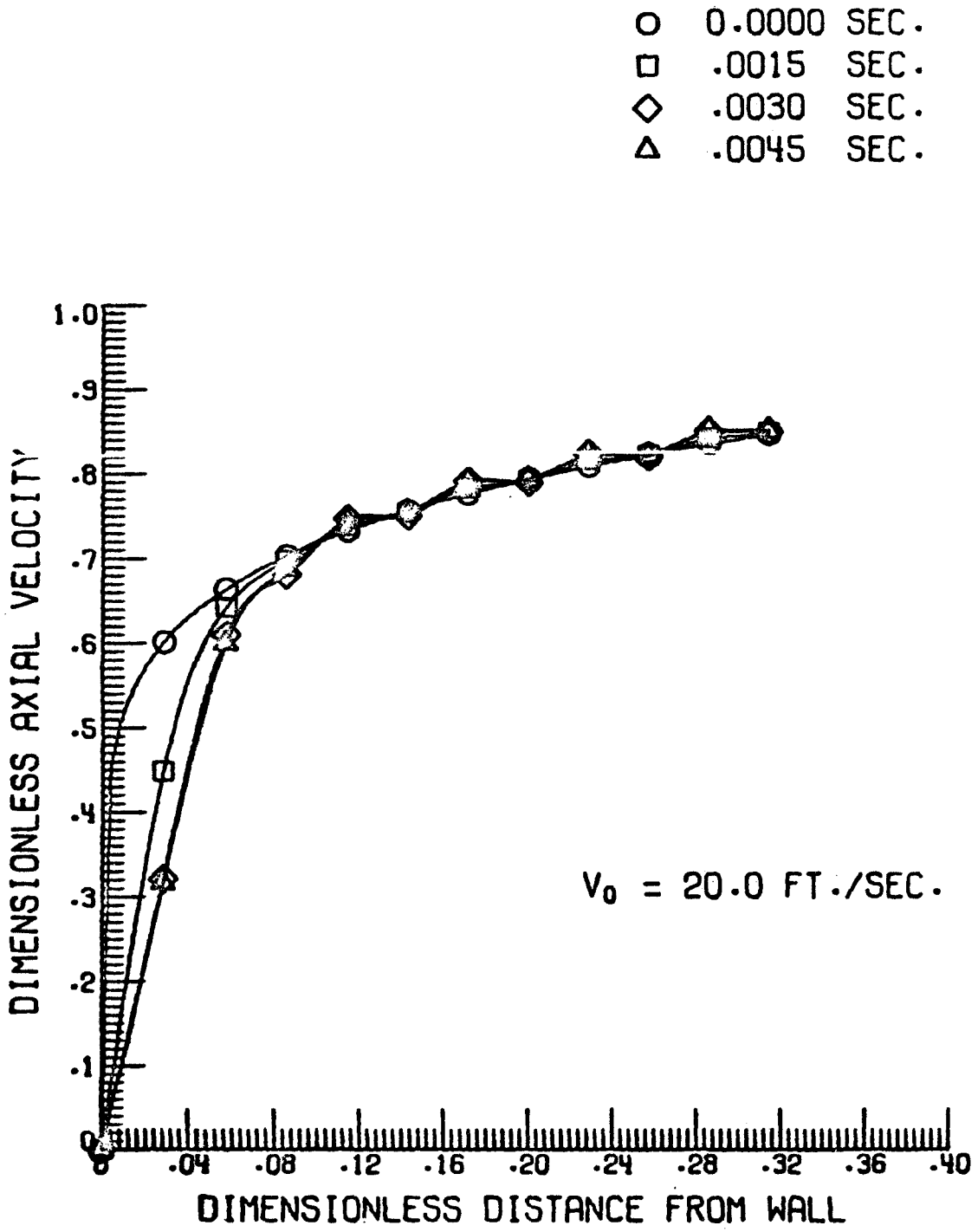
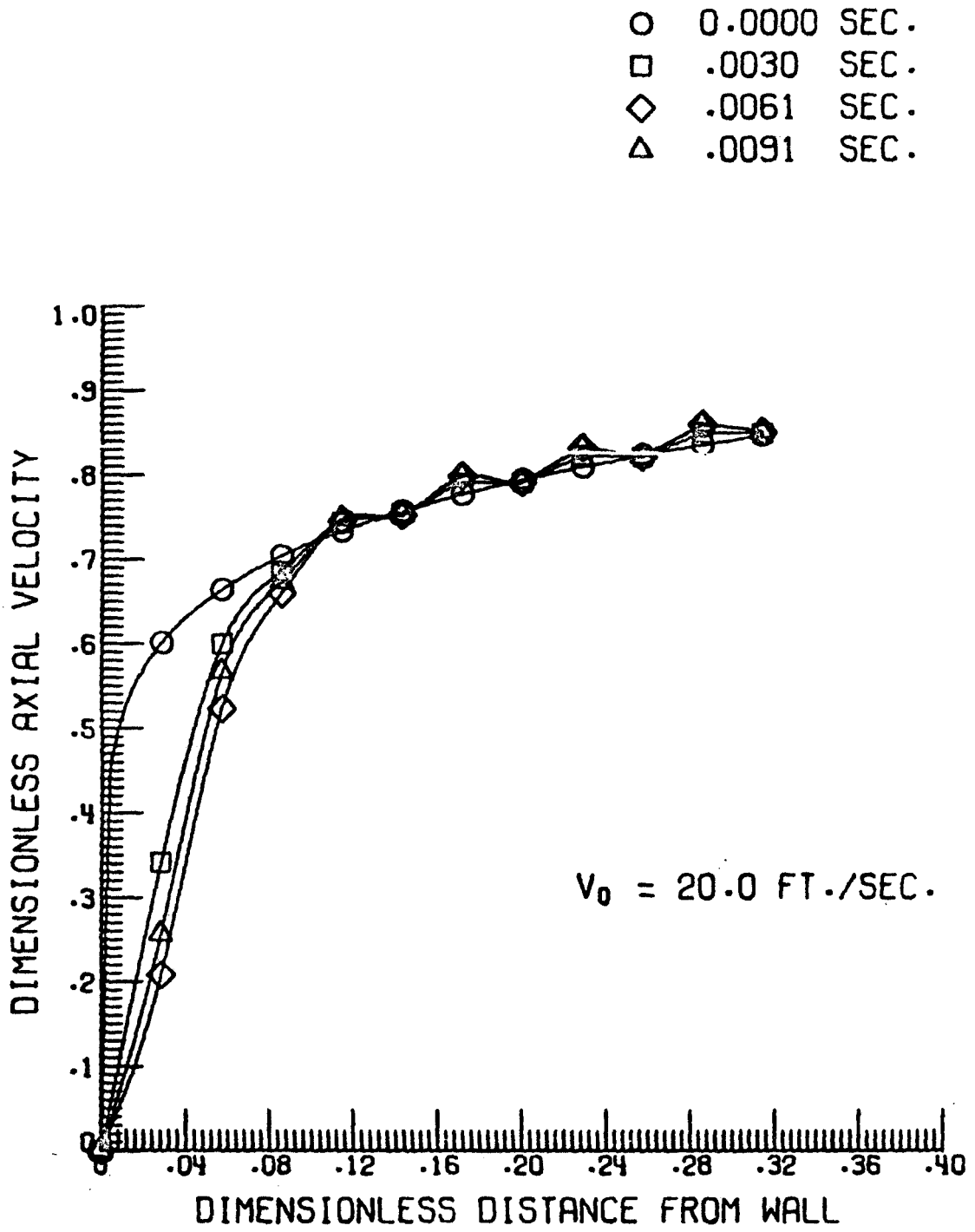


FIGURE (VII-9.3)
PROFILE AT AXIAL POSITION. $\hat{Z}$ = .36 .
IN GAS PHASE



The steady-state profiles of all the dependent variables are plotted in Figure VII-10.1 - VII-10.8. There is a decrease in the density of the mixture corresponding to an increase in the gas phase temperature in the axial direction. A sharp temperature peak to correspond to a sustaining flame is indicated at $\hat{z} = 0.36$. The magnitude of the axial velocity gradient at the fuel surface decreases in the axial direction as mass addition and combustion are more dominant in that direction. Since the vaporization process is assumed to be the mechanism for the mass addition of fuel, the radial velocity component is expected to approach zero in the close vicinity of the fuel surface. With the coarse grid spacing used, the finite difference method can only approximate the solution by values fluctuating around zero. This fluctuation propagates into the downstream flow and what is observed in Figure VII-10.4 is really a phenomenon due to the finite difference approximation. These fluctuating values for the radial velocity component in turn produce the ripples observed in Figures VII-10.1 - VII-10.3. This also indicates that the density, the gas phase temperature and the axial velocity component are strongly coupled to the radial velocity component. The sum of the mass fractions of aluminum, oxygen and aluminum oxide at any grid point should add up to unity and this is remarkably obeyed within the convergence criteria used. A pronounced production of Al_2O_3 with the corresponding depletion of aluminum and oxygen can be observed in the sustaining flame zone at $\hat{z} = 0.36$. Since a steady-state temperature profile in the solid phase is assumed initially at the start of the combustion process, the solution for the temperature in the solid phase is trivial. There is, however, a

Figure VII-10.1 - VII-10.8 Steady-State Profile of all the Dependent Variables at Axial Position, $\hat{Z}$ = 0.00, 0.12, 0.24 and 0.36

FIGURE (VII-10.1)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

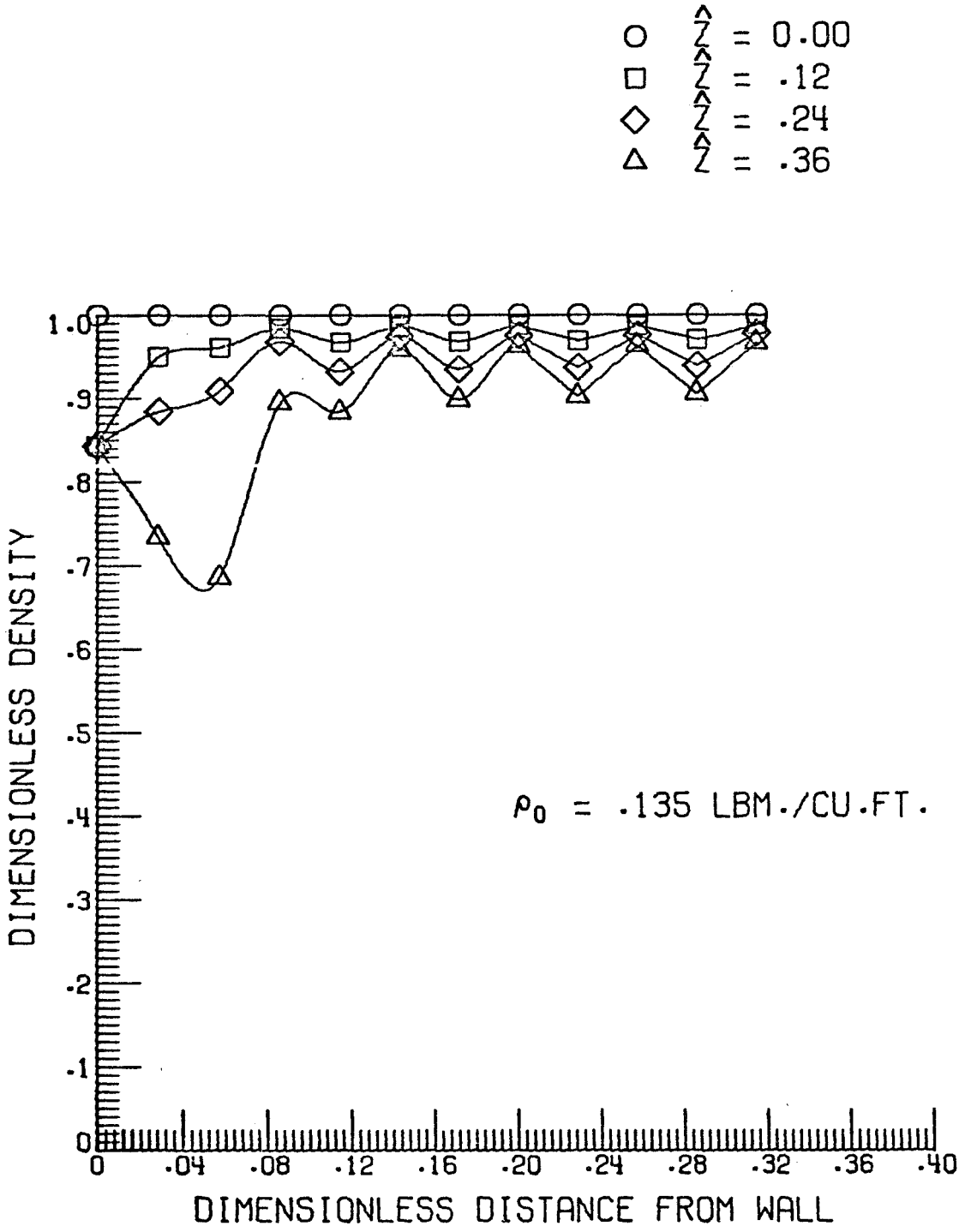


FIGURE (VII-10.2)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

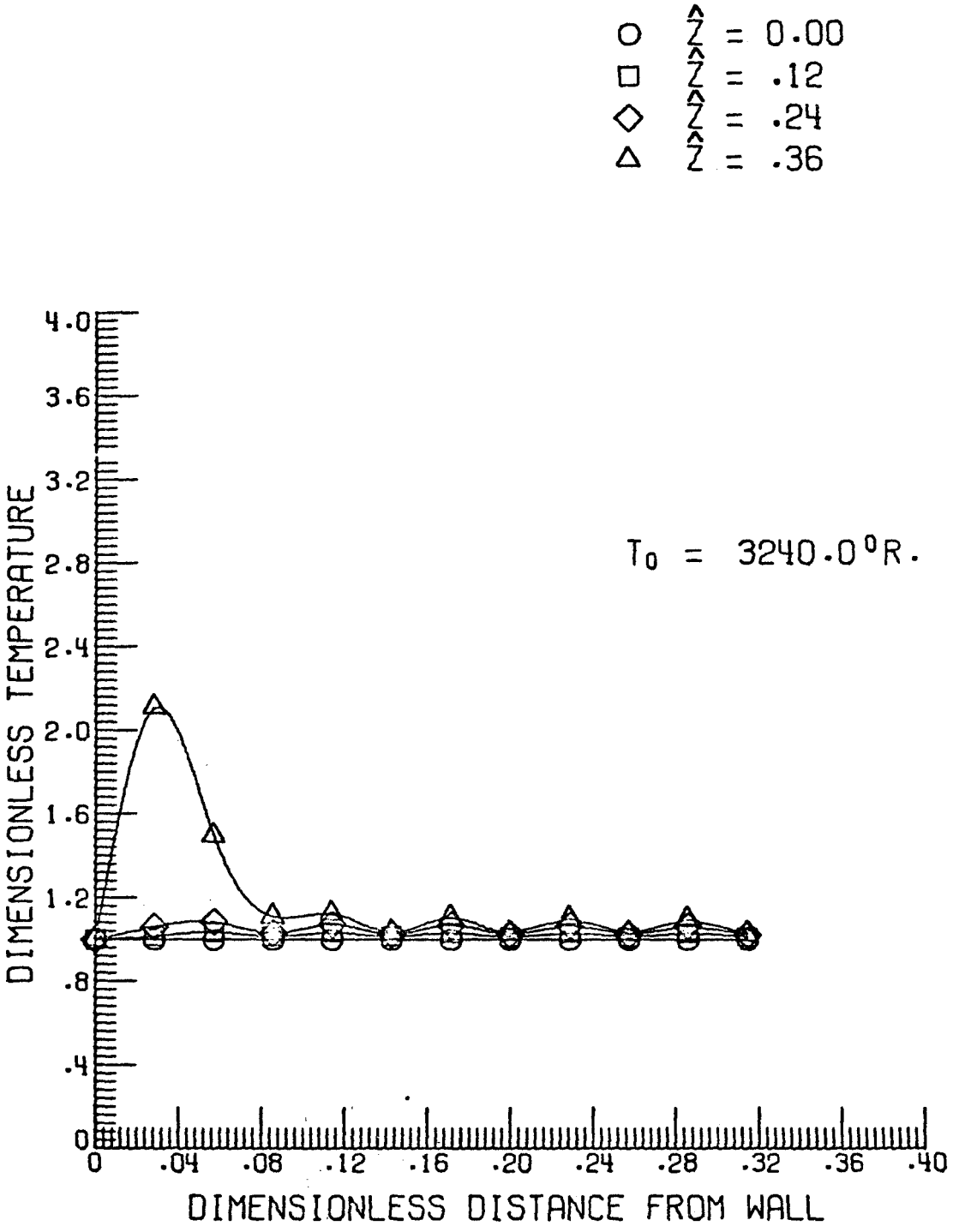


FIGURE (VII-10.3)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

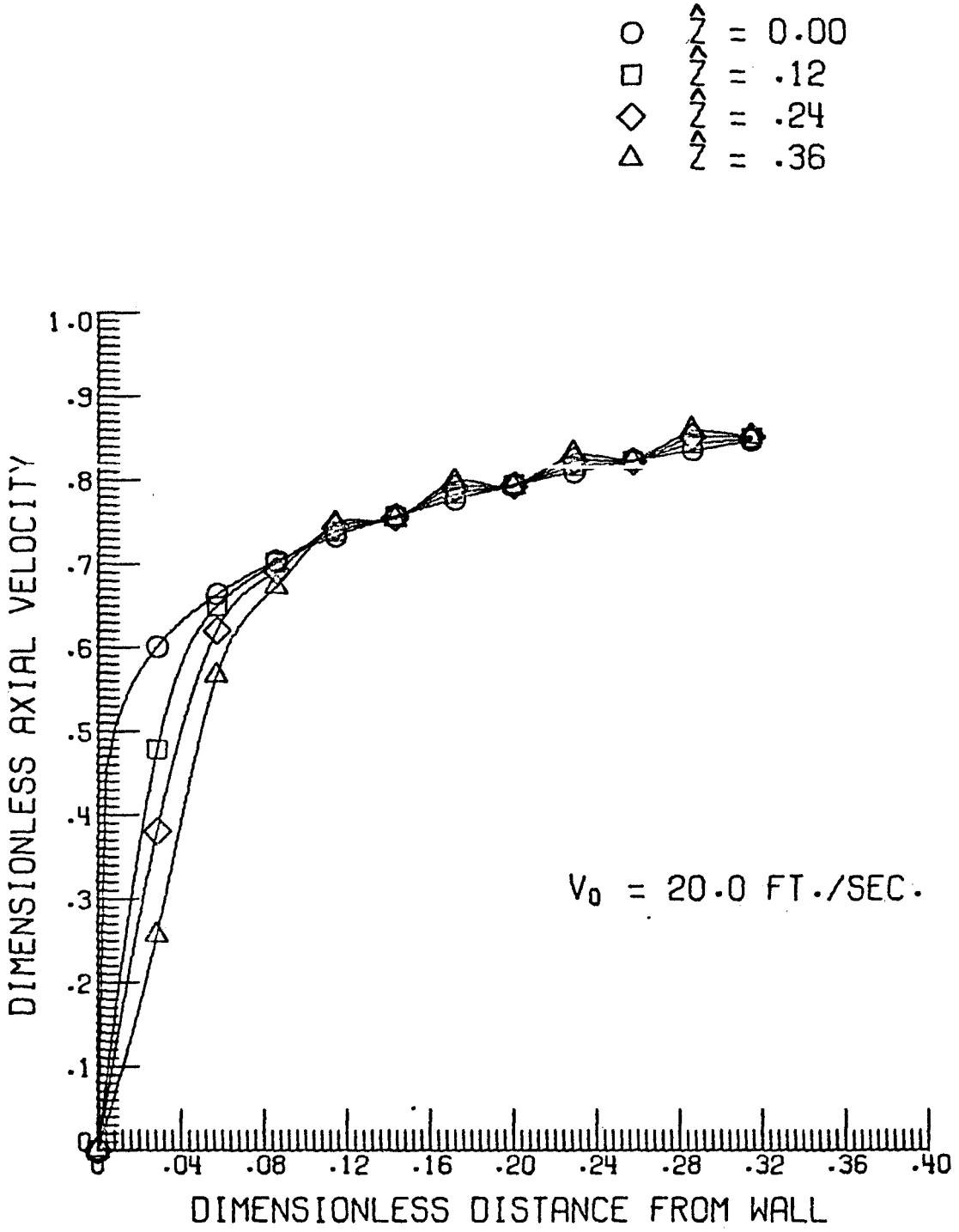


FIGURE (VII-10.4)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

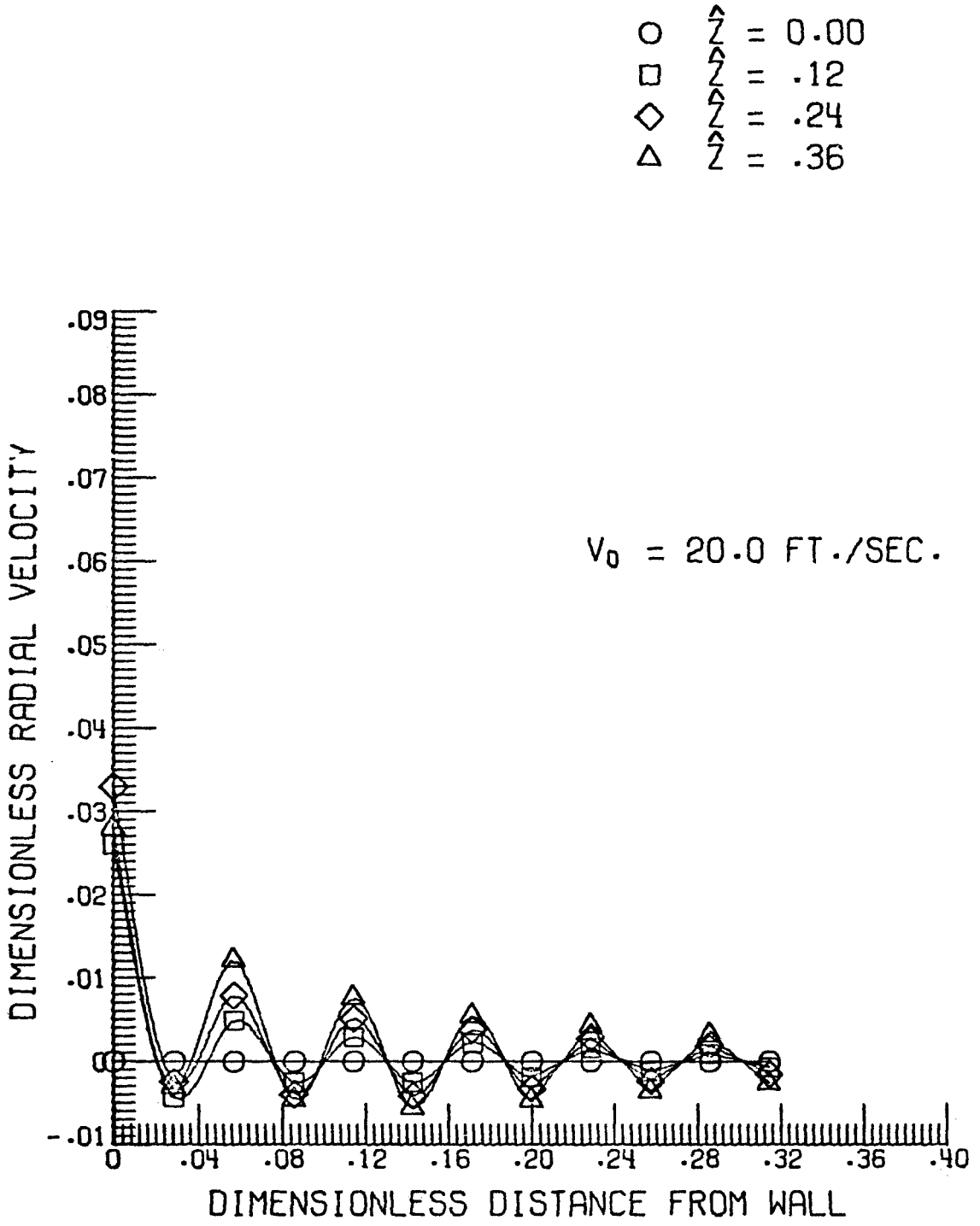


FIGURE (VII-10.5)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

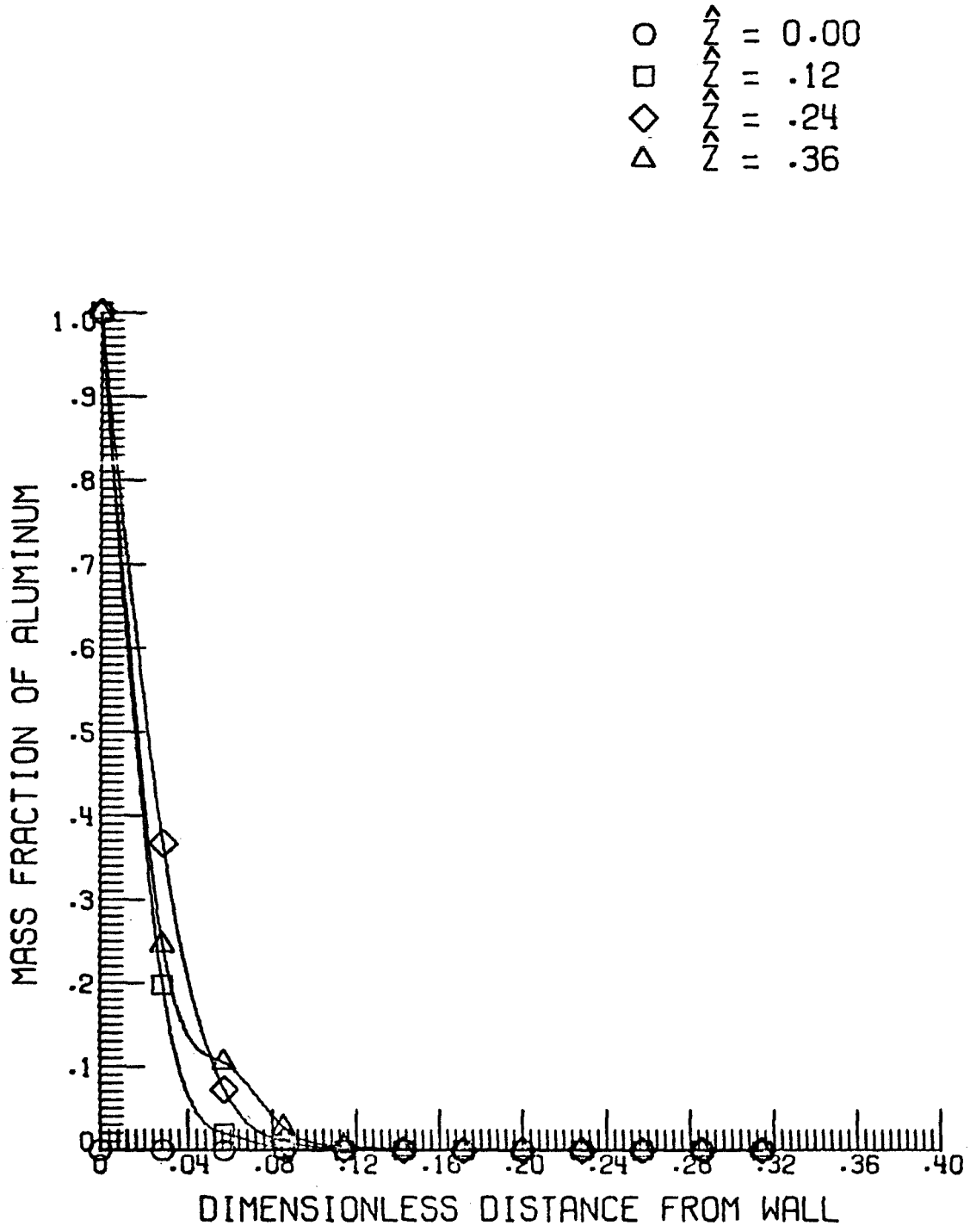


FIGURE (VII-10.6)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

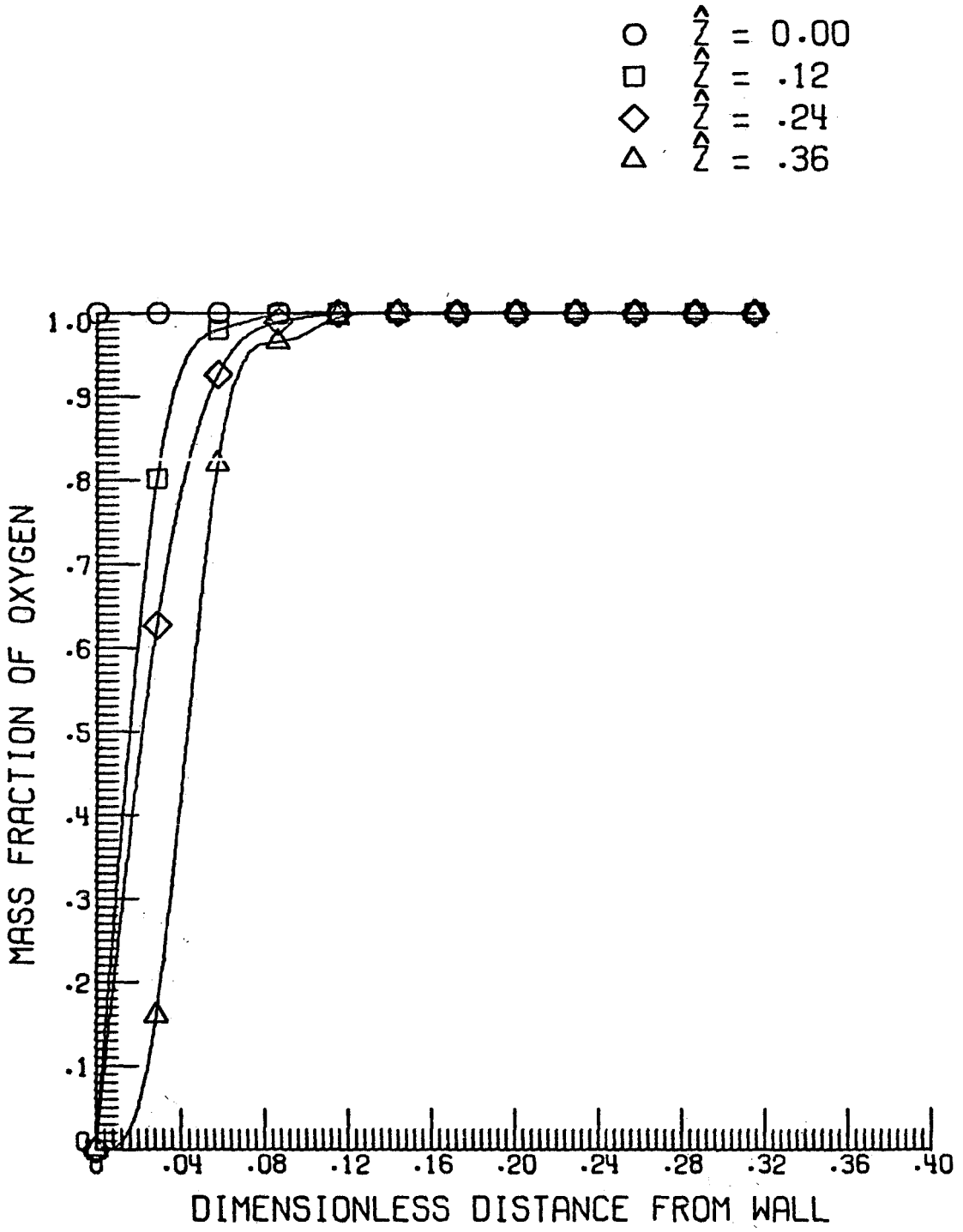


FIGURE (VII-10.7)
PROFILE AT TIME = .00915 SEC.
IN GAS PHASE

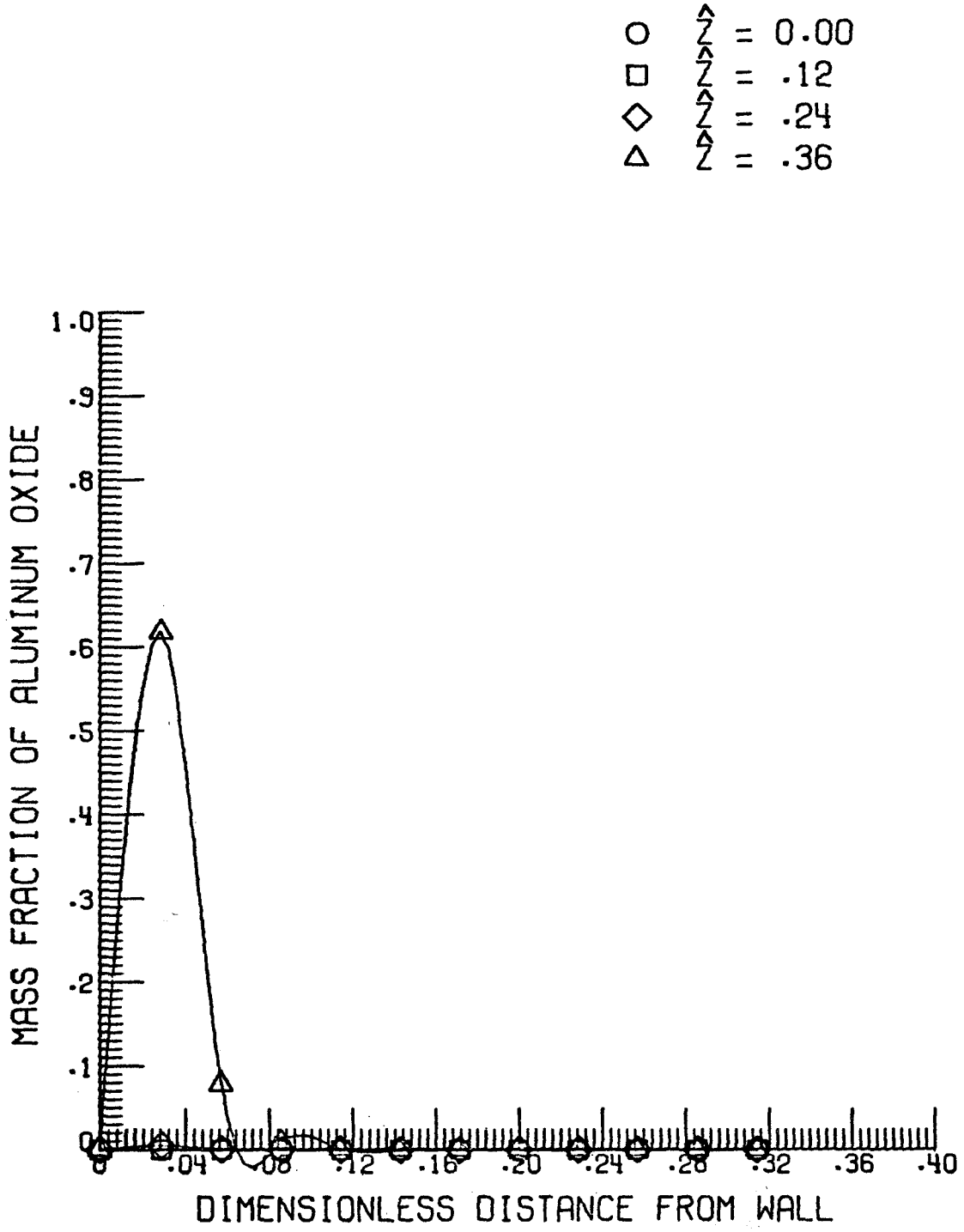
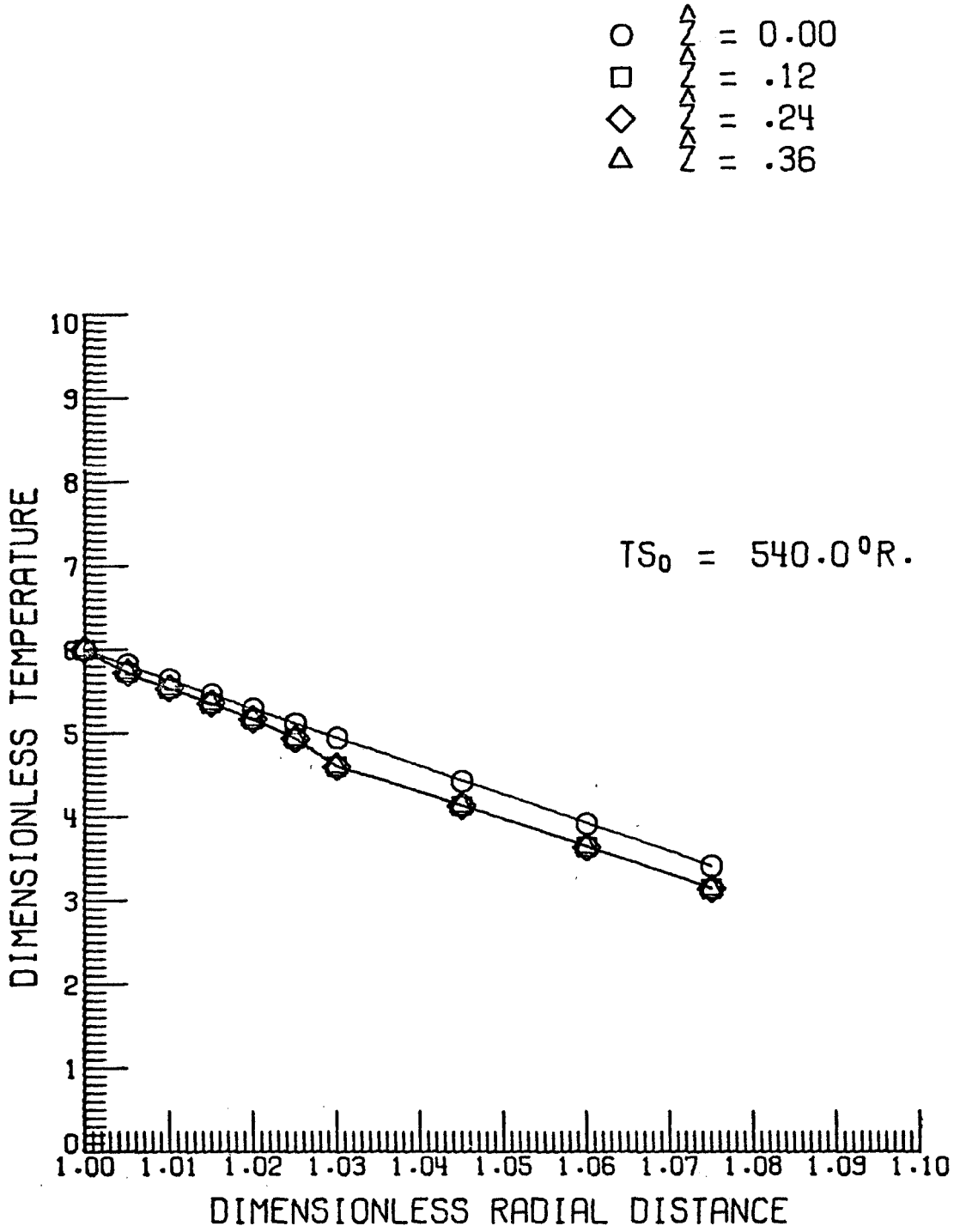


FIGURE (VII-10.8)
PROFILE AT TIME = .00915 SEC.
IN SOLID PHASE



maximum of about 7% difference between the calculated and the initially assumed values. This is due to the inherent approximation in the difference equation when the option of two regions of uniform grid spacing in the solid phase is used.

CHAPTER VIII

CONCLUSIONS

An overall approach has been followed to study the heterogeneous combustion processes in hybrid rocket systems through the use of numerical computational methods. The achievements in return for the efforts put forth can be summarized as follows:

(a) A computational method has been developed which is capable of solving the complete set of transient, two-dimensional, conservation equations for a reacting gas mixture.

(b) It has been further demonstrated that this system of equations is capable of handling the heterogeneous combustion problem resulting from the turbulent flow of an oxidizer over solid fuel.

(c) The transient solutions obtained indicate a smooth transition from initial to steady-state conditions, allowing a study of the transient phenomena in heterogeneous combustion processes to be made within a reasonable amount of computing time.

(d) The calculated results indicate that a flame is formed very close to the fuel surface, and, that there is a decrease in the magnitude of the axial velocity gradient at the fuel surface.

(e) The steady-state conditions achieved indicate good qualitative agreement with available experimental data.

(f) It has been found as initially expected that the neglect of radiative heat transfer is unrealistic, and so, radiative heat transfer effect should be included in future study of hybrid rocket systems.

(g) With the development of more sophisticated theoretical models, it is expected that this computational method can be used to simulate experimental conditions more realistically.

CHAPTER IX

RECOMMENDATIONS FOR FUTURE WORK

The work presented in the previous chapters are only the beginning of an ambitious undertaking. The numerical solution of the set of general, two-dimensional, conservation equations as presented in Chapter III even for a simple case has opened a new horizon in the area of computational physics. In order that this computational method can be used to simulate experimental conditions, more realistic models need to be formulated and incorporated into the current computer program. A number of these future work items are described below.

A. Variable Mass Addition from Fuel Surface

(a) Description: An investigation into the effect of variable rate of mass addition from fuel surface. A constant rate is currently being used.

(b) Discussion: From published literature, it is evident that the fuel surface regression rate in a hybrid rocket system is variable. Assuming that the fuel surface chemical reaction is primarily a function of the temperature at the gas-solid interface, T_w, the fuel surface pyrolysis rate can be expressed in the Arrhenius form as follows:

$$\dot{r} = A \exp \left[\frac{-E_s}{RT_w}\right] \qquad \text{(IX.1)}$$

where A and E_s are empirical constants. From experimental regression rate data, the constants A and E_s can be evaluated.

B. Radiative Heat Transfer

(a) Description: An investigation into the effects due to radiative heat transfer from the hot gases to the fuel surface. This is currently neglected.

(b) Discussion: When metallic fuel is employed in a hybrid rocket system, maximum temperature in the combustion chamber can range anywhere from 3000°K to 4000°K. Radiative heat transfer from the hot combustion flame to the fuel surface can no longer be neglected. Assuming that a gray-body equilibrium description applies, an additional term to account for radiative heat transfer effects can be included in the energy balance equation at the interface.

C. Variable Properties

(a) Description: An investigation into the effects of temperature and position dependence of variable fluid and transport properties. Constant properties are currently used.

(b) Discussion: Since turbulent flow and extreme temperature gradient are characteristic of a hybrid rocket system, the effect of variable fluid and transport properties will be studied. The specific heat per unit mass at constant pressure for the chemical species in the gas phase is generally temperature dependent and can be fitted to experimentally measured data through the use of empirical equation as follows:

$$C_{pi} = a_i + b_i T + c_i T^2 \qquad \text{(IX.2)}$$

where a_i, b_i and c_i are empirical constants. Values of these constants

have been reported by Kobe (58) for a number of gases commonly encountered in the petrochemical industry.

In experimental studies of combusting turbulent boundary layers, both Kulgein (59) and, Jones and Isaacson (46) have concluded that there is no evidence of combustion-induced turbulence. Hence, the eddy viscosity derived for isothermal flow can be used for chemical reacting flow. Based on an extension of Prandtl's mixing length theory, Williamson (60) derived an expression for the eddy viscosity in isothermal, fully established channel flow. Thus, the dimensionless viscosity, $\hat{\mu}$, can be expressed after some manipulation as a function primarily of the dimensionless position coordinate, $\hat{r}$, as follows:

$$\hat{\mu} = 0.021\hat{\rho}(Re)^{\frac{7}{8}} (\hat{r})^{\frac{1}{2}} (1 - \hat{r})\exp[\hat{r}] \qquad (IX.3)$$

Jones <u>et. al.</u> (61) reported that it is reasonable to assume that the eddy diffusivity is equal to the eddy viscosity. Hence, the dimensionless binary diffusion coefficient, $\hat{D}_i$, can be expressed as follows:

$$\hat{D}_i = 0.021 \left(\frac{r_o v_o}{D_o}\right)(Re)^{-\frac{1}{8}} (\hat{r})^{\frac{1}{2}} (1 - \hat{r})\exp[\hat{r}] \qquad (IX.4)$$

If it is further assumed that the eddy thermal diffusivity is equal to the eddy viscosity, a position dependent expression for the dimensionless thermal conductivity can be derived.

D. Improved Turbulence Model

(a) Description: Development of a turbulent transport model utilizing perturbation theory to include fluctuation flow. Currently, a time-averaged turbulent model is used, which differs from the laminar flow model only in the magnitude of the transport coefficients.

(b) Discussion: Since flow in a hybrid rocket system is highly turbulent, the effect due to turbulence intensity may play an important role. This effect can be studied through the perturbation theory. With the addition of transport terms due to fluctuation, the current governing equations in the gas phase are the zero order perturbation equations. The first order perturbation equations have to be derived for computer use.

E. Complex Chemical Kinetics

(a) Description: An investigation into the effects of complex chemical kinetics, in which realistic reaction chains will be used. A simple one-step overall irreversible chemical reaction is currently used.

(b) Discussion: Most gas-phase chemical reactions cannot be described by a simple one-step stoichiometric relation. As the reaction proceeds, a number of steps are involved in which chemical species, that do not appear in the final products, take part. To describe such a complex reaction, these intermediate species have to be included. This involves a study of the reaction mechanisms. From the postulated reaction mechanisms, the result is a set of elementary reactions represented by the following equation:

$$\sum_{\ell=1}^{L} \nu'_{\ell_i} \left[\frac{\rho y_i}{M_i}\right] \overset{k_\ell}{\rightarrow} \sum_{\ell=1}^{L} \nu''_{\ell_i} \left[\frac{\rho y_i}{M_i}\right] \qquad \text{(IX.5)}$$

The rate of change of concentration of a particular chemical species can then be derived from this set of elementary reactions.

F. Physical Recession Effects

(a) Description: Investigation of the effects due to a physically receding fuel surface. Currently, the fuel surface geometry remains fixed although a regression rate of fuel is assumed.

(b) Discussion: In an actual hybrid rocket system, the geometry of the combustion chamber changes continuously as the fuel surface recedes. This internal geometric variation will directly affect the static pressure. Therefore, cases will arise where the current computer program is unrepresentative, and does not permit comparisons to be made with test results. Major reprogramming will be required.

G. Field Plotting

(a) Description: Development of a new plotting program to produce easily read field plots. Currently, computer program PLOT is used to plot axial profiles of all the dependent variables.

(b) Discussion: The current plotting program can be used to study the transient phenomena of reactive fluid flow. However, in order to facilitate easy interpretation of computed results in terms of qualitative trends and to get an overall picture of the entire flow field, a new plotting program to generate field plots of all the dependent variables at any instant of time should be developed. A continuous display

of field plots on oscilloscope through real time assimilation will be equivalent to performing a theoretical experiment of reactive flow in a hybrid rocket system.

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APPENDIX A

VERIFICATION OF THE CRANK-NICOLSON SCHEME

Analytical solutions for steady-state, two-dimensional heat conduction in a rectangular plate have been used to verify the implicit Crank-Nicolson scheme for the transient heat conduction equation. The plate is assumed to be homogeneous with a thermal conductivity of 10 Btu/hr.ft.°F, a diffusivity of 0.20 sq.ft./hr., a length L = 0.096 ft. and a width d = 0.024 ft. Consider the rectangular plate shown in Figure A.1. Two sides of the plate are insulated, one side is maintained at a constant temperature, T_o, and the remaining side has a temperature distribution, f(z), impressed upon it. Assuming that the temperature distribution varies linearly from T_o = 300°F at z = d to T_{max} = 800°F at z = 0, f(z) can then be expressed as follows:

$$f(z) = (T_{max} - T_o)(1 - \frac{z}{d}) + T_o \qquad \text{(A-1)}$$

The governing equation is

$$\frac{\partial^2 T}{\partial z^2} + \frac{\partial^2 T}{\partial x^2} = 0 \qquad \text{(A-2)}$$

Let $\theta = T - T_o$ and $F(z) = f(z) - T_o = \theta_{max}(1 - z/d)$, then, equation (B-2) becomes

$$\frac{\partial^2 \theta}{\partial z^2} + \frac{\partial^2 \theta}{\partial x^2} = 0 \qquad \text{(A-3)}$$

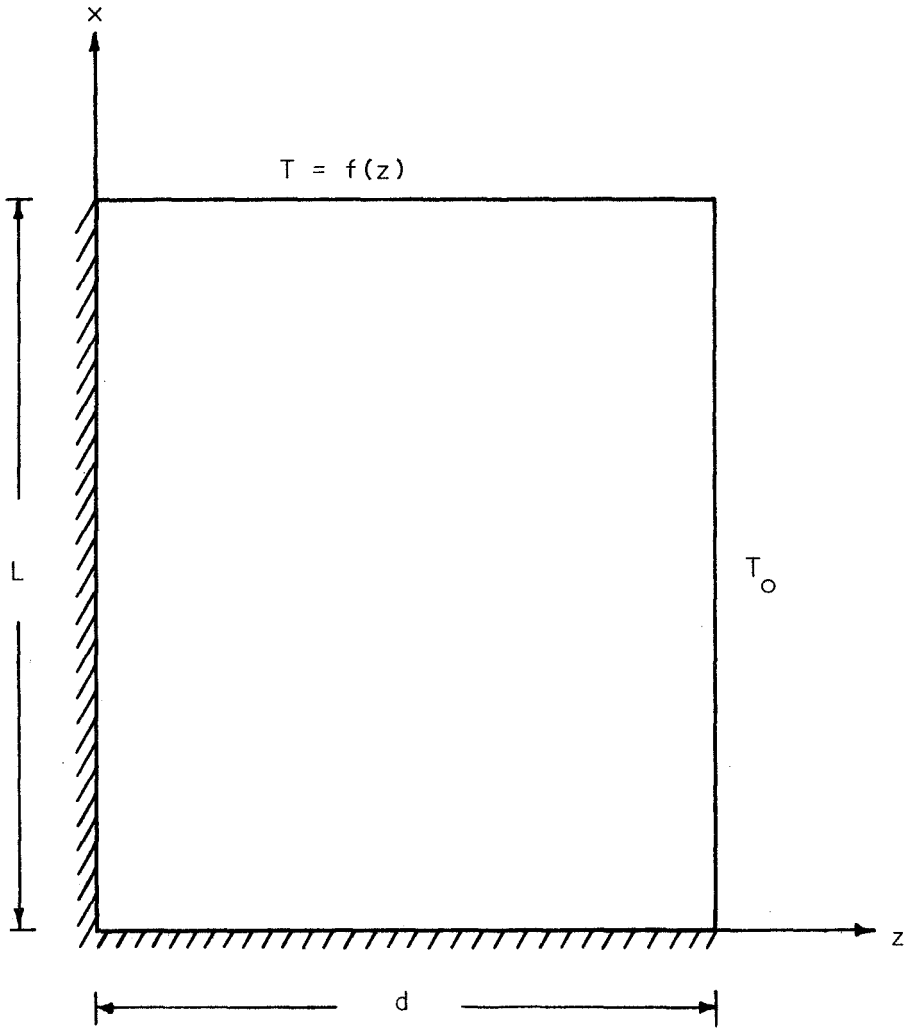

Figure A.1 Two-Dimensional Heat Conduction in a Rectangular Plate

Boundary conditions are as follows:

(a) $\frac{\partial\theta}{\partial z} = 0$ at $z = 0$;

(b) $\theta = 0$ at $z = d$;

(c) $\frac{\partial\theta}{\partial x} = 0$ at $x = 0$;

(d) $\theta = F(z)$ at $x = L$.

The solution to the differential equation (A.3) with the given boundary conditions has been derived as follows:[1]

$$\theta(z_1 x) = \sum_{n=0}^{\infty} \frac{8\theta_{max}}{(2n+1)^2} \frac{\cosh[\frac{(2n+1)\pi x}{2d}]}{\cosh[\frac{(2n+1)\pi L}{2d}]} \cos[\frac{(2n+1)z}{2d}] \qquad (A.4)$$

The sum of the series as represented by equation (A.4) has been solved by computer[2] and the isotherms for every 100 degrees can be drawn as shown in Figure A.2.

Using the Crank-Nicolson scheme as described in Chapter IV, equation (III.10) has been used to obtain solution for the transient, two-dimensional heat conduction in the same rectangular plate. A square grid of 0.006 ft and a time increment, $\Delta t = 0.0075$ sec. have been chosen. In order to

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[1]Hung, W. S. Y., Term Problem for M.E. 231a-Heat Transmission, Dept. of Mech. Engr., Stanford University, Stanford, California, 1965.

[2]Ibid.

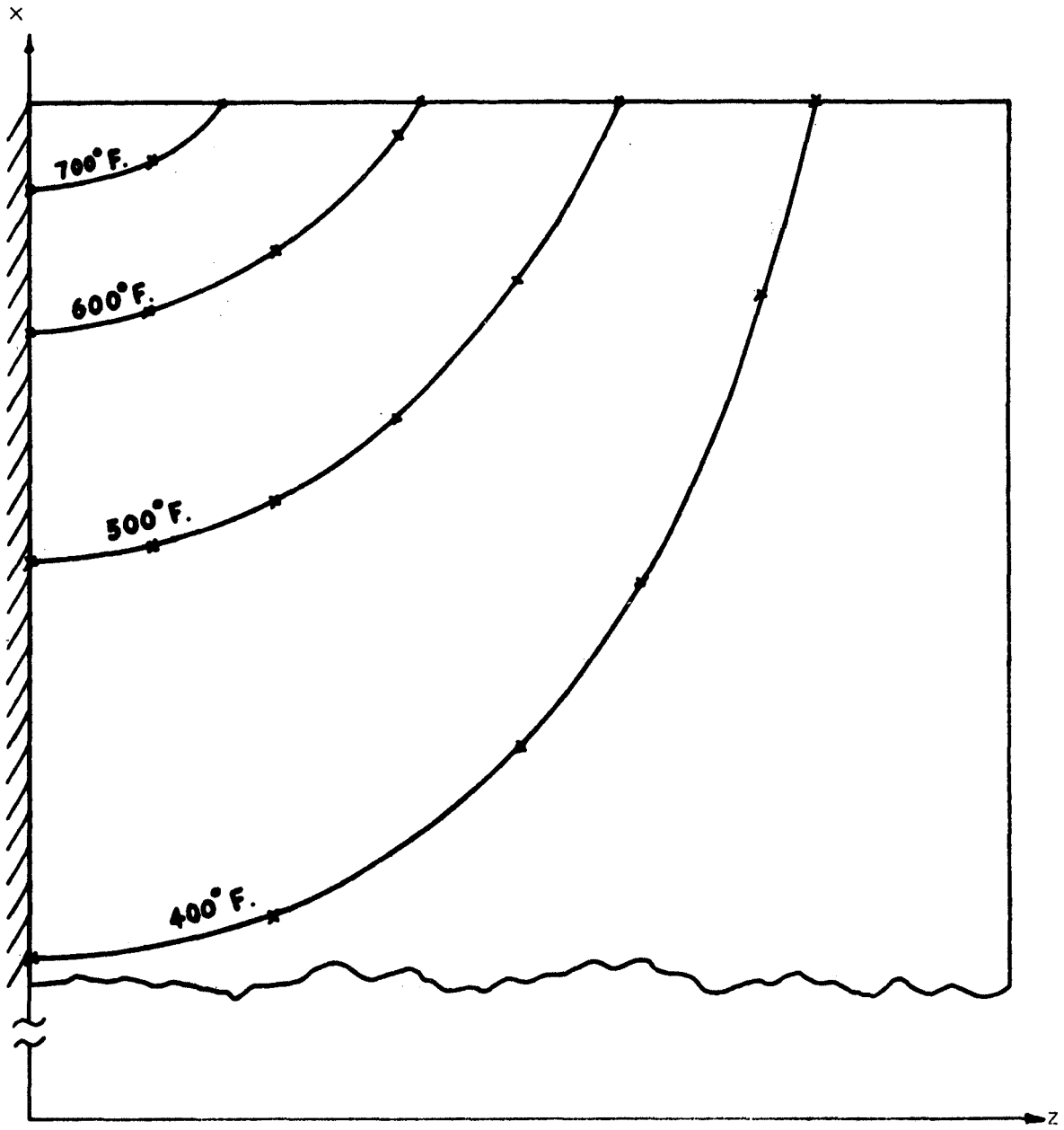


Figure A.2 Isothermal Lines in the Rectangular Plate

eliminate the effect due to curvature, the dimensionless radius, $\hat{r}$, has been set arbitrarily as 100,000. From a plot of temperature versus time for the grid point where maximum temperature change occurred, as shown in Figure A.3, it can be observed that the temperature distribution approached the steady-state condition in approximately 9 seconds. The results of the analytical series solution and of the transient numerical solution at the end of 9 seconds are tabulated as shown in Table A.1 and Table A.2 respectively. A maximum error of 2.07% has been calculated. This is within the truncation error for the analytical series solution. Thus, it has been verified that the difference equation for equation (III.10) is correct.

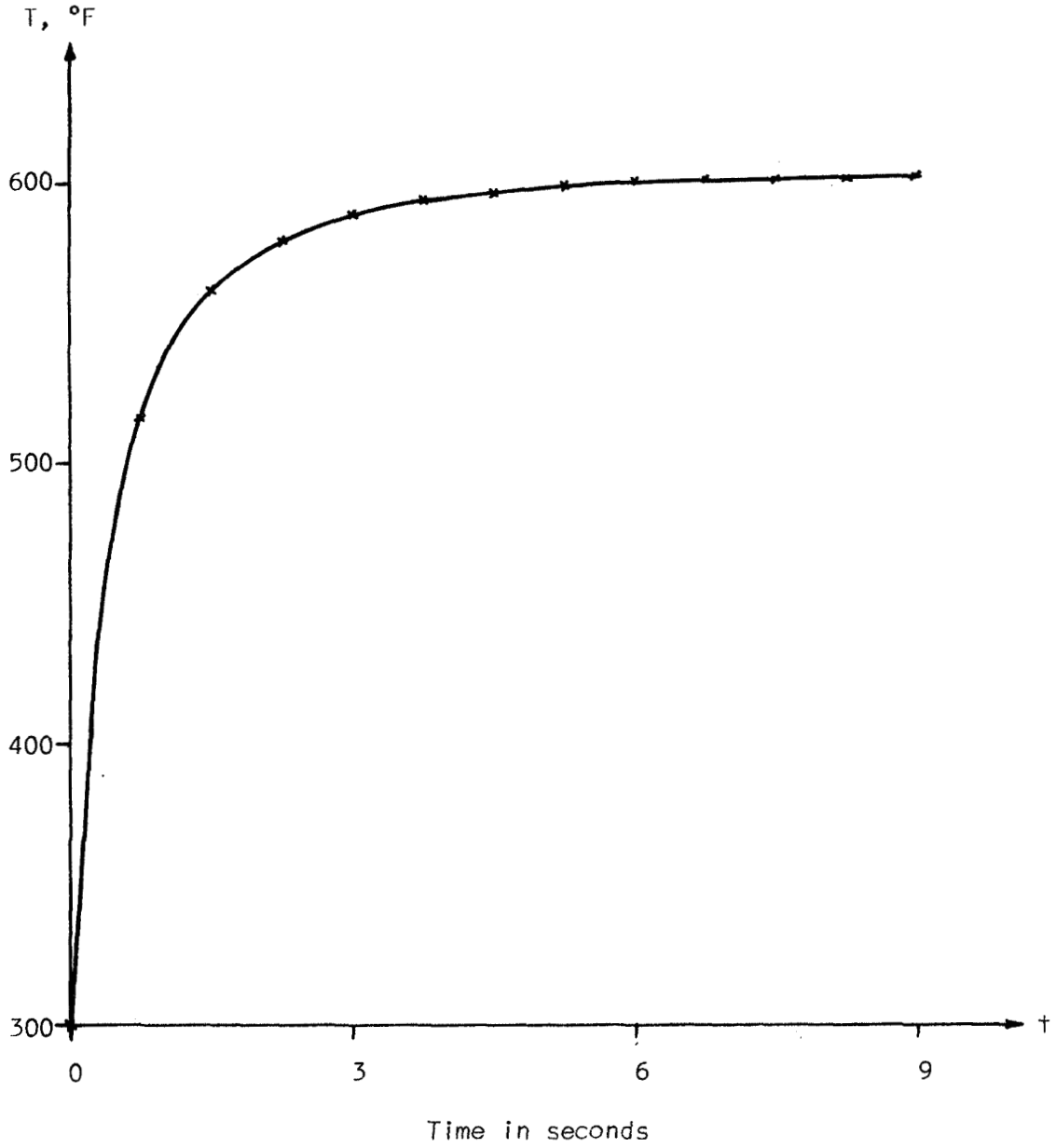


Figure A.3 Temperature Versus Time at z = 0, x = 0.09 ft.

Table A.1 Temperature (°F) in the Rectangular Plate Shown in Figure A.1 - Solution by Equation (A.4)

x(ft.) \ z(ft.)	0.0	.006	.012	.018	.024
.084	797.5	675.0	550.0	425.0	300.0
.078	590.5	556.6	482.5	393.8	300.0
.072	489.4	472.2	427.5	367.1	300.0
.066	426.1	415.8	387.3	346.6	300.0
.060	384.7	378.0	359.3	331.9	300.0
.054	357.0	352.6	340.1	321.7	300.0
.048	338.5	335.5	327.1	314.7	300.0
.042	326.0	324.0	318.3	309.9	300.0
.036	317.5	316.2	312.4	306.7	300.0
.030	311.8	310.9	308.4	304.5	300.0

Table A.2 Temperature (°F) in the Rectangular Plate Shown in Figure A.1 - Transient Solution of Equation (III.10) by an Implicit Crank-Nicolson Scheme at t = 9 sec.

x(ft.) \ z(ft.)	0.0	.006	.012	.018	.024
.084	800.1	675.0	549.9	425.1	300.0
.078	602.7	558.6	482.4	393.6	300.0
.072	494.4	474.0	427.5	366.6	300.0
.066	427.8	386.4	387.0	346.2	300.0
.060	384.3	377.4	358.5	331.2	300.0
.054	355.2	351.0	338.7	320.7	300.0
.048	336.0	333.3	325.5	313.8	300.0
.042	322.1	321.3	316.5	308.7	300.0
.036	314.7	313.5	310.5	305.7	300.0
.030	309.3	308.4	306.6	303.6	300.0

APPENDIX B

PROGRAM HETCOMB

This computer program has been developed to perform a theoretical study of heterogeneous combustion in an idealized hybrid rocket chamber. The conservation equations derived in Chapter III are solved by using the finite-difference schemes described in Chapter IV. The convergence criteria and iterative procedures employed have been described in Chapter V. This computer program allows either uniform radial grid spacing or two regions of uniform grid spacing in both the gas and the solid phases. In the axial direction, however, only uniform grid spacing is allowed. Furthermore, this computer program allows the transient calculation to proceed in an unlimited number of runs through the use of magnetic tapes until the steady-state condition has been reached. The nomenclature of the important symbols used and a general flow chart for this computer program is presented first. The input arrangement is described and a sample input is shown. The type and form of the output are discussed. A sample input is included for the purpose of checking out the computer program. The storage requirement and the time limit to be specified are discussed. A listing of the computer program are included at the end of the appendix.

A. Nomenclature

A listing of the important symbols used in computer program HETCOMB is defined as follows:

AD = Absolute difference between calculated and guess values of any of the dependent variables at any grid point;

AE = Allowed total relative errors for any of the dependent variables at any time step, η;

ALAM = Dimensionless thermal conductivity in gas phase;

ALAMO = Characteristic thermal conductivity in gas phase, Btu/hr/ft/°R;

ALAMRA = Ratio of the characteristic thermal conductivity in solid phase to that in the gas phase;

ALAMS = Dimensionless thermal conductivity in solid phase;

ALAMSO = Characteristic thermal conductivity in solid phase, Btu/hr/ft/°R;

ALPHAO = Characteristic thermal diffusivity in gas phase.

ALPHASO = Characteristic thermal diffusivity in solid phase.

AMAX = Maximum allowed difference between calculated and guess values of any of the dependent variables at any grid point, ζ;

AMI = Molecular weight of species, I, lb_m/mole;

AMIN = Allowed minimum absolute value;

AMU = Dimensionless viscosity in gas phase;

AMUO = Characteristic viscosity in gas phase, lb_m/ft/sec;

ANU1 = Stoicheiometric coefficient of oxidizer;

ANU2 = Stoicheiometric coefficient of fuel;

ANU3 = Stoicheiometric coefficient of product;

CAI = Constant, a_i, for the evaluation of C_{pi}, Btu/lb_m;

CBI = Constant, b_i, for the evaluation of C_{pi}, Btu/lb_m;

CCI = Constant, c_i, for the evaluation of C_{pi}, Btu/lb_m;

CE = Activation energy, Kcal/g-mole;

CP = Dimensionless specific heat per unit mass at constant pressure;

CPO = Characteristic specific heat per unit mass at constant pressure, Btu/lb_m/°R;

CSO = Characteristic specific heat per unit mass in solid phase, Btu/lb_m/°R;

CPI = Dimensionless specific heat per unit mass at constant pressure of species, I;

DO = Characteristic binary diffusion coefficient in gas phase;

DAM = $\frac{RO\ WO}{DENO\ VO}$;

DI1,DI2 = Dimensionless binary diffusion coefficient of species, I;

DELR = Dimensionless radial grid spacing in gas phase;

DELR1 = Dimensionless radial grid spacing in region 1 of gas phase;

DELR2 = Dimensionless radial grid spacing in region 2 of gas phase;

DELRS = Dimensionless radial grid spacing in solid phase;

DELRS1 = Dimensionless radial grid spacing in region 1 of solid phase;

DELRS2 = Dimensionless radial grid spacing in region 2 of solid phase;

DELT = Dimensionless time increment;

DELZ = Dimensionless axial grid spacing;

DEN = Dimensionless density at any grid point in gas phase;

DENO = Characteristic density in gas phase, lb_m/cu.ft;

DENRA = DENSO/DENO;

DENS = Dimensionless density at any grid point in solid phase;

DENSO = Characteristic density in solid phase, lb_m/cu.ft;

DFURA1 = $\frac{DO}{RO\ VO}$;

DFURA2 = $\frac{DO}{ALPHAO}$;

DFURA3 = $\frac{RO\ VO}{ALPHAO}$;

DFURA4 = $\frac{RO\ VO}{ALPHASO}$;

DFURA5 = $\frac{RO\ RRO}{ALPHASO}$;

EC = Eckert number;

FLL = Lower flammability limit;

FUL = Upper flammability limit;

HIO = Characteristic enthalpy per unit mass in the gas phase, Btu/lb_m;

HI1,HI2 = Dimensionless enthalpy per unit mass of species, I, in the gas phase;

HLG = Heat of vaporization of species, I, Btu/lb_m;

HSGI = Dimensionless heat of sublimation of fuel at interface;

HSL = Heat of fusion of species, I, Btu/lb_m;

L = Time step counter;

LL = Number of time-step calculations before calculated values of all the dependent variables are printed out;

K = Counter during convergence test: 1 for TS, 2 for VR, 3 for VZ, 4 for T, 5 for mass fraction of oxidizer, 6 for mass fraction of fuel and 7 for mass fraction of product;

M = Radial grid number in gas phase;

MS = Radial grid number in solid phase;

N = Axial grid number;

NI = Number of chemical species present in the gas phase;

NIT = Number of iterations allowed;

NR = Grid position in the gas phase when radial grid size is changed;

NRS = Grid position in the solid phase when radial grid size is changed;

NT = Total number of time-step calculations for any particular run;

NX = DELR1/DELR2;

NXS = DELRS2/DELRS1;

NW = Total number of radial grids in the gas phase;

NWS = Total number of radial grids in the solid phase;

NZ = Total number of axial grids;

P = Dimensionless pressure at any grid point in the gas phase;

PG = Imposed favorable downstream pressure gradient, psf/ft;

PR = Prandtl number;

R = Dimensionless radius;

RO = Characteristic radius, ft;

RA1 = Molecular radius of oxidizer;

RA2 = Molecular radius of fuel;

RE = Reynolds number;

ROF = Reaction order for fuel;

ROO = Reaction order for oxidizer;

RR = Dimensionless regression rate of fuel at interface

RRO = Characteristic regression rate of fuel, ft/sec;

RS = Dimensionless radius in the solid phase;

SC = Schmidt number;

SF = Steric factor;

T = Dimensionless temperature at any grid point in the gas phase;

TO = Characteristic temperature in the gas phase, °R;

TBP = Boiling point of species I, °R;

TC = Minimum temperature for combustion to take place;

TEMPR = Calculated values for the dimensionless radial velocity;

TEMPS = Calculated values for the dimensionless temperature in the solid phase;

TEMPT = Calculated values for the dimensionless temperature in the gas phase;

TEMPY = Calculated values for the mass fraction of chemical species, I;

TEMPZ = Calculated values for the dimensionless axial velocity;

TIME = Dimensionless time;

TRA = TO/TSO;

TS = Dimensionless temperature at any grid point in the solid phase;

TSO = Characteristic temperature in the solid phase, °R;

TSC = Minimum temperature for the fuel to vaporize, °R;

VO = Characteristic velocity in the gas phase, ft/sec;

VR = Dimensionless radial velocity at any grid point in the gas phase;

VRA = RRO/VO;

VZ = Dimensionless axial velocity at any grid point in the gas phase;

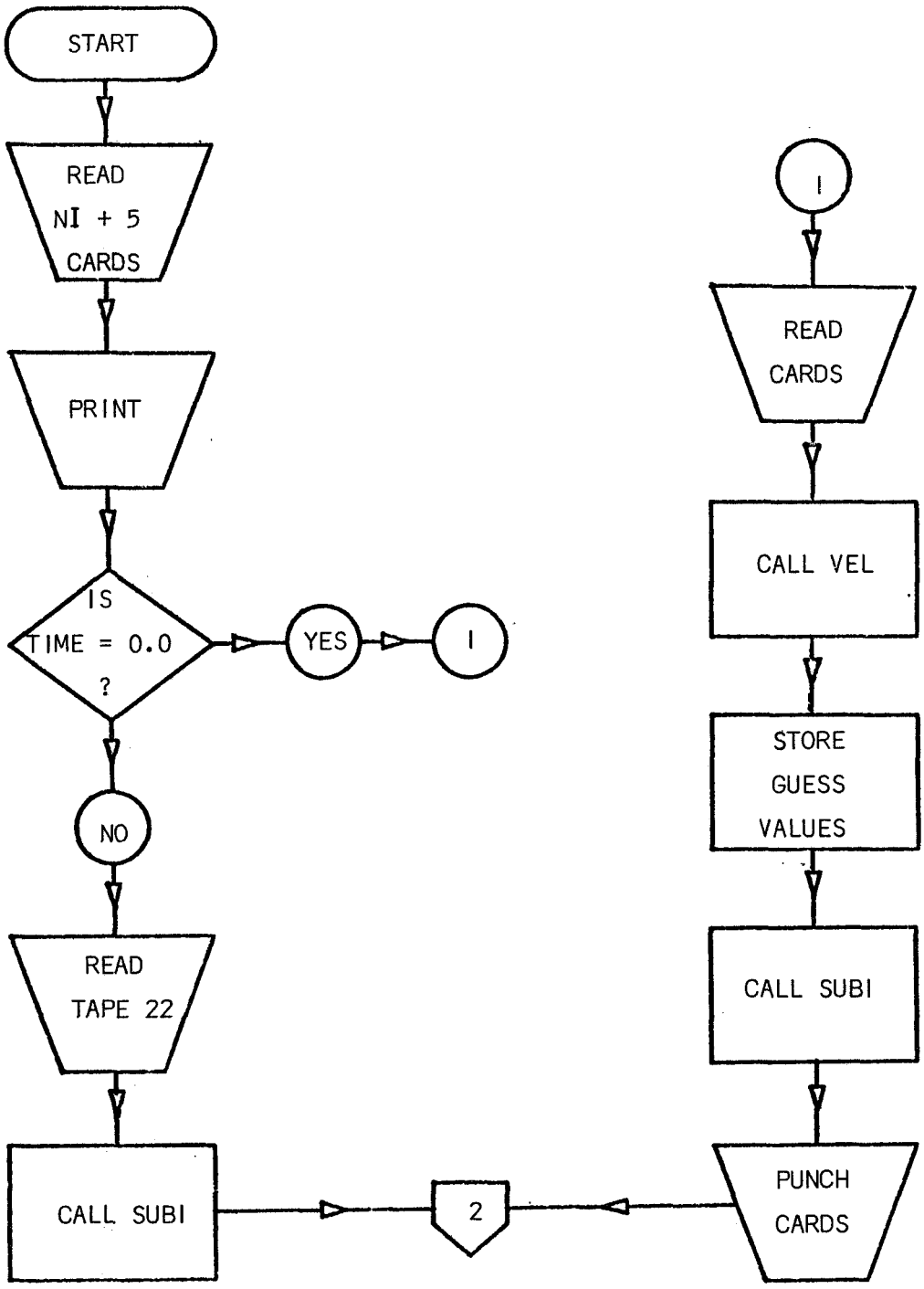
WO = Characteristic species production rate, lb_m/cu.ft/sec;

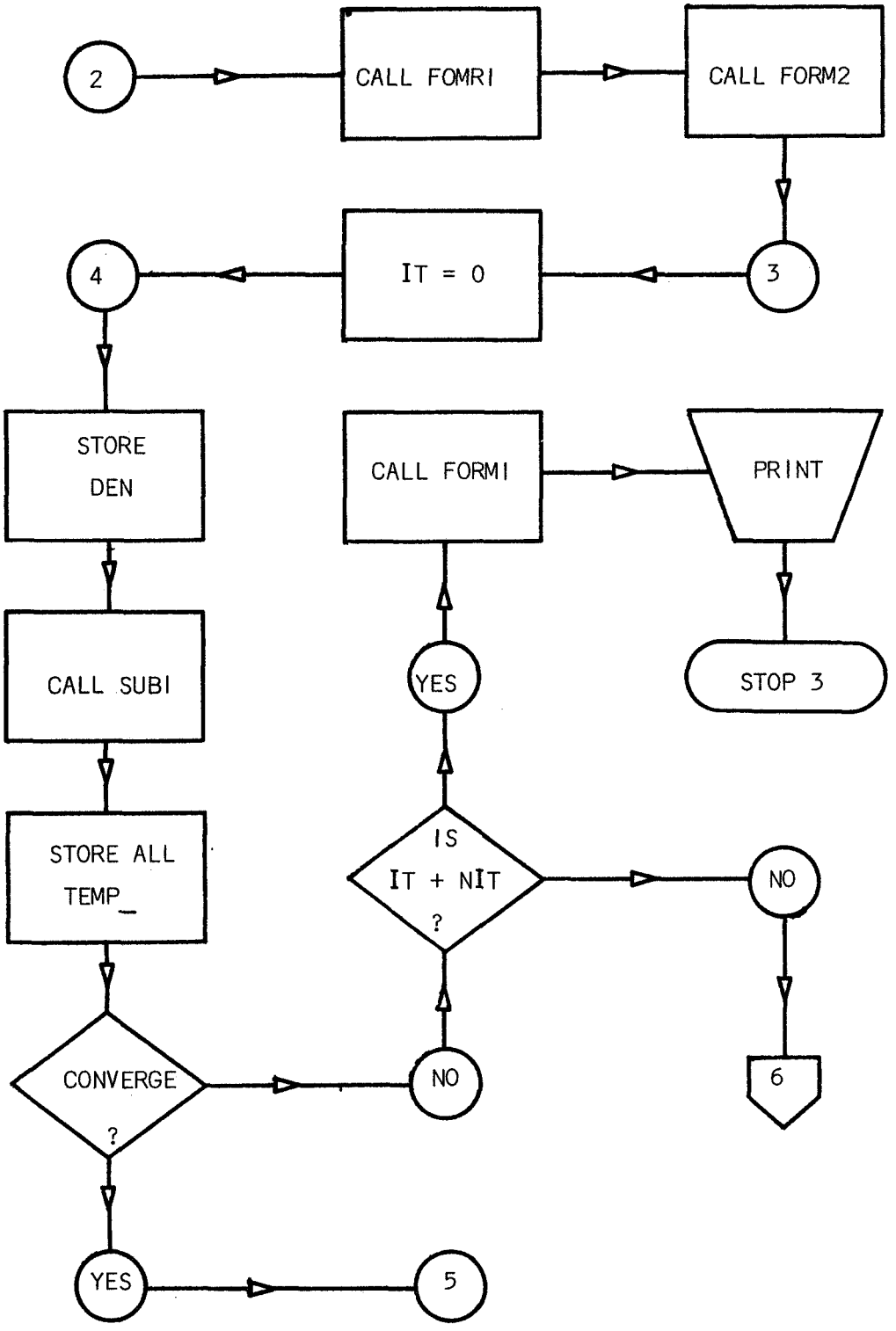
WI1,WI2 = Dimensionless rate of production of species at any grid point in the gas phase;

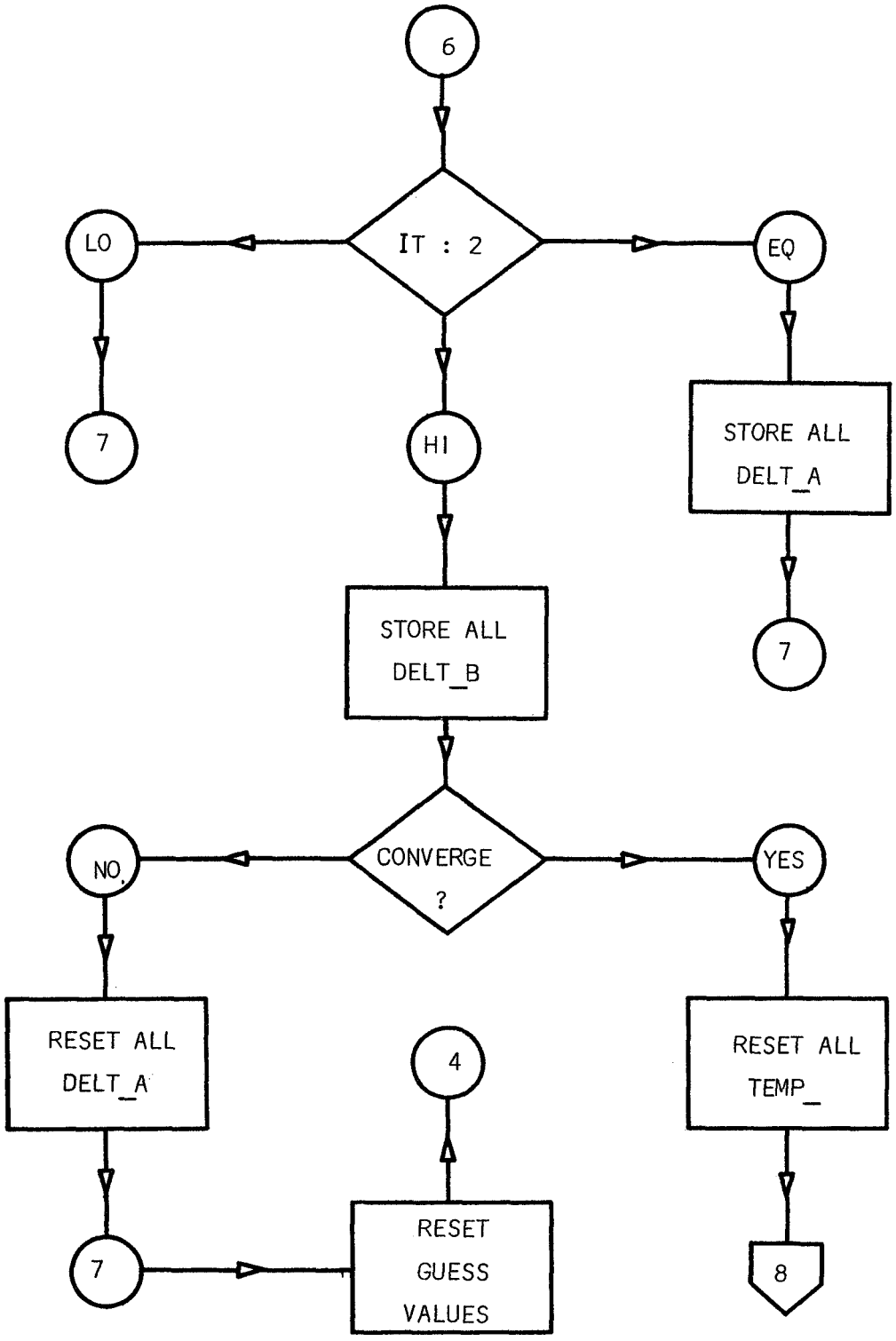
YI1,YI2 = Mass fraction of chemical species, I, at any grid point in the gas phase.

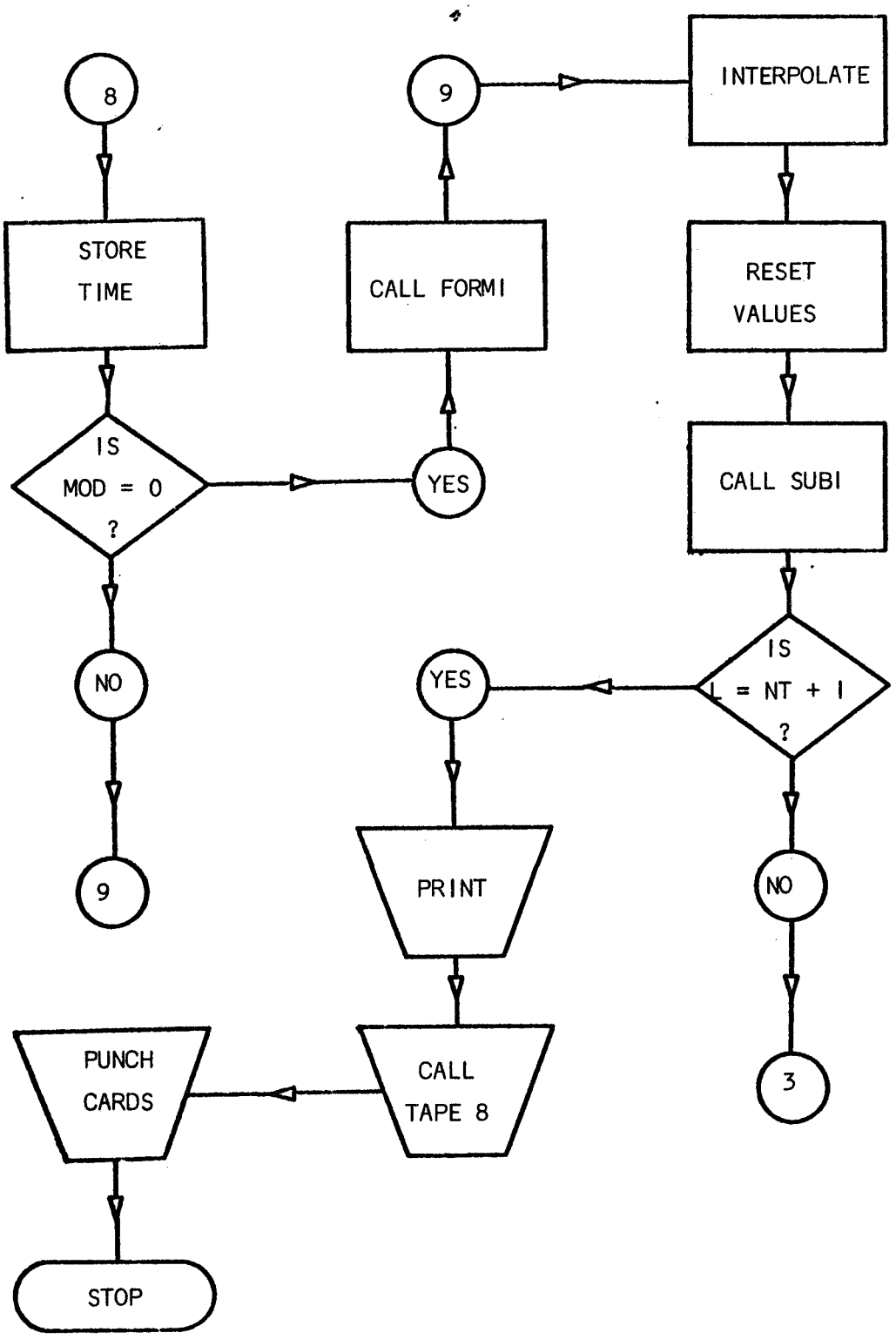
B. Flow Chart

A diagram to show the main logic of computer program HETCOMB is presented in the form of a flow chart as follows:


START
READ
NI + 5
CARDS
PRINT
IS
TIME = 0.0
?
YES
1
NO
READ
TAPE 22
CALL SUBI
2
1
READ
CARDS
CALL VEL
STORE
GUESS
VALUES
CALL SUBI
PUNCH
CARDS


2
CALL FOMRI
CALL FORM2
3
IT = 0
4
STORE
DEN
CALL FORMI
PRINT
CALL SUBI
YES
STOP 3
STORE ALL
TEMP_
IS
IT + NIT
?
NO
CONVERGE
?
NO
6
YES
5


6
IT : 2
LO
EQ
7
HI
STORE ALL
DELT_A
STORE ALL
DELT_B
7
CONVERGE
?
NO
YES
RESET ALL
DELT_A
4
RESET ALL
TEMP_
7
RESET
GUESS
VALUES
8


8
STORE TIME
IS MOD = 0 ?
YES
NO
9
9
CALL FORMI
INTERPOLATE
RESET VALUES
CALL SUBI
IS L = NT + 1 ?
YES
NO
3
PRINT
CALL TAPE 8
PUNCH CARDS
STOP

C. Input to Program HETCOMB

For initial run, only input cards are used. For continued run, both input cards and magnetic tape are employed. The input arrangement is as follows:

1. The first input card contains 11 numbers punched according to the format (11I4). These numbers are called by the following symbols: NW, NWS, NZ, NR, NRS, NX, NXS, NI, NIT, NT, LL. They are defined as follows:

   NW = Total number of radial grids in the gas phase;

   NWS = Total number of radial grids in the solid phase;

   NZ = Total number of axial grids;

   NR = Grid position in the gas phase when radial grid size is changed;

   NRS = Grid position in the solid phase when radial grid size is changed;

   NX = Ratio of radial grid sizes for the two uniform regions in the gas phase, DELR1/DELR2;

   NXS = Ratio of radial grid sizes for the two regions in the solid phase, DELRS2/DELRS1;

   NI = Number of chemical species present in the gas phase;

   NIT = Number of iterations allowed in any time step;

   NT = Total number of time-step calculations for any particular run;

   LL = Number of time-step calculations before calculated values of all the dependent variables are printed out.

   In this program, the maximum values for NW, NWS, NZ and NI are 20, 15, 10 and 3 respectively. The general grid layout is fixed by assigning proper values to the first seven numbers: NW, NWS, NZ, NR, NRS, NX, NXS. Grid spacing in the axial direction is uniform. However, the

following options are available for grid spacing in the radial direction:

(a) NR ≥ NW : Uniform radial grid spacing in the gas phase;

(b) NR < NW : Two regions of uniform radial grid spacing in the gas phase;

(c) NRS ≥ NWS: Uniform radial grid spacing in the solid phase;

(d) NRS < NWS: Two regions of uniform radial grid spacing in the solid phase.

Options (b) and (d) allow the use of finer radial grid spacing in the vicinity of the gas-solid interface. When options (b) and (d) are employed, NX and NXS define the relationship between the radial grid spacing in the gas phase and the solid phase respectively. A sketch is drawn as shown in Figure B.1 to illustrate the interrelationship between these first seven numbers when options (b) and (d) are used in the general grid layout. For continued run, the first eight numbers should be the same as the initial run. The last three numbers, NIT, NT and LL, can be varied for any particular run. However, if LL should be greater than NT in any run, calculated values of the dependent variables will not be printed out.

2. The second input card consists of 7 numbers punched according to the format (6F10.0,E10.0). These numbers are called by the following symbols: DELRS, DELZ, DELT, AE, AMAX, TIME, and AMIN. They are defined as follows:

DELRS = Dimensionless radial grid spacing in the solid phase;

DELZ = Dimensionless axial grid spacing;

DELT = Dimensionless time increment;

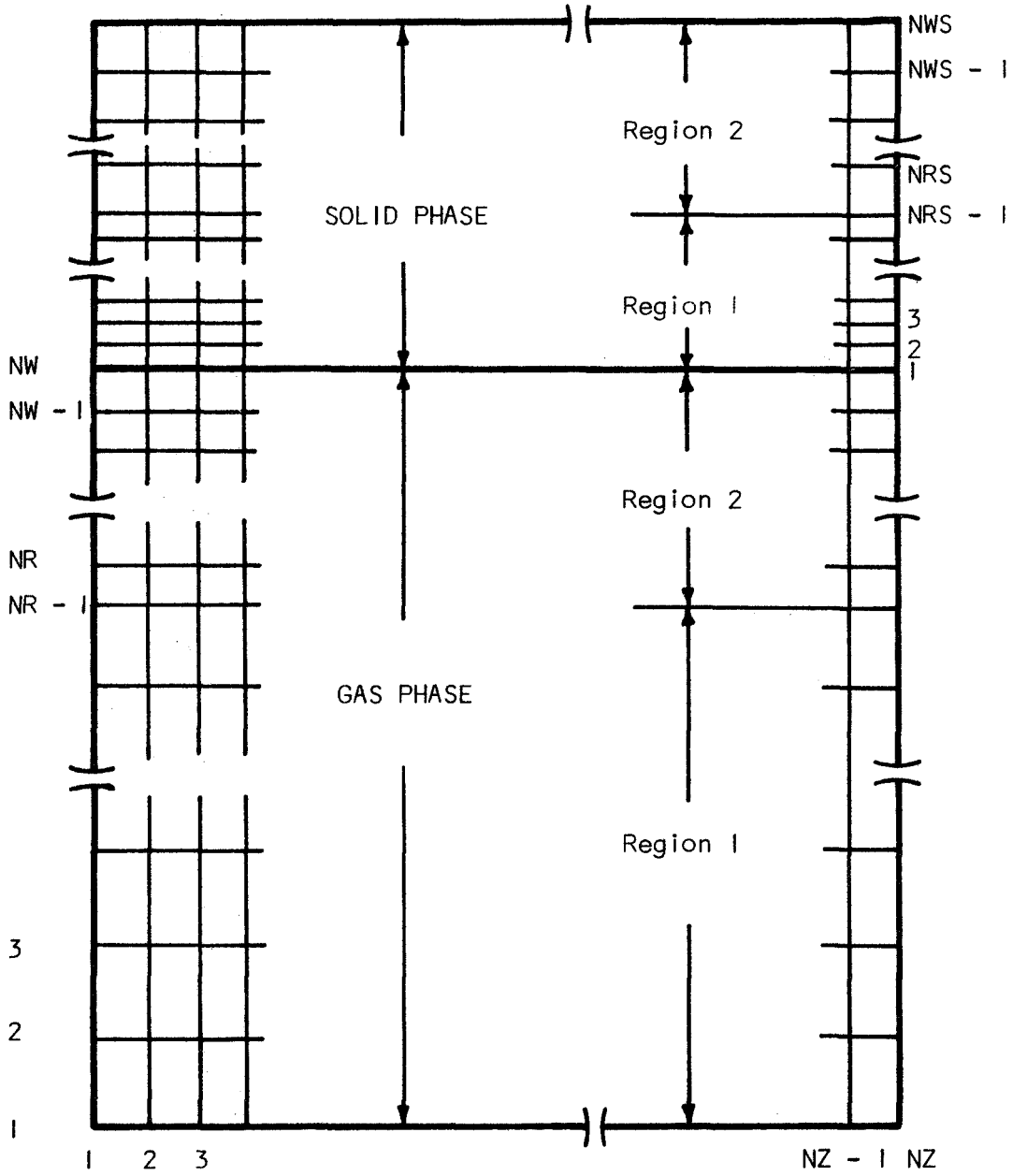


Figure B.1 General Grid Layout

AE = Allowed total relative errors for any of the dependent variables in any time step;

AMAX = Maximum allowed difference between calculated and guess values of any of the dependent variables at any grid point;

TIME = Total time elapsed, sec.;

AMIN = Allowed minimum absolute value.

Since the current model assumes a constant radius for the combustion chamber, the size for the dimensionless radial grid spacing in the gas phase, DELR, can be calculated when values have been assigned to NW, NR and NX. For NR ≥ NW:

$$DELR = \frac{1}{NW - 1} .$$

For NR < NW:

$$DELR2 = \frac{1}{NW - NR + 1 + NX(NR - 2)} ,$$

and

$$DELR1 = (NX)(DELR2),$$

where DELR1 and DELR2 are the corresponding values for DELR in regions 1 and 2 in the gas phase respectively. The dimensionless radial grid spacing in the solid phase is read in as the first number in this input card. For NRS ≥ NWS: DELRS1 = DELRS2 = DELRS. For NRS < NWS: DELRS1 = DELRS and DELRS2 = (NXS)(DELRS) where DELRS1 and DELRS2 are the corresponding values for DELRS in regions 1 and 2 in the solid

phase respectively. In order to eliminate round-off error, the value for DELT is assigned as a negative integer power of two. This negative integer value is read in as DELT and the program will be reassigned a value for DELT as follows:

$$DELT = (2.0)^{DELT}.$$

For initial run, a value of 0.0 is assigned to TIME; for continued run, any value other than 0.0 is assigned to TIME. For continued run, the values assigned to DELRS, DELZ, AE, AMAX and AMIN should be identical with those of the corresponding initial run.

3. The third input card consists of 10 numbers punched according to the format (10F8.0). These numbers are called by the following symbols: RO, VO, TO, DENO, AMUO, DO, WO, ALAMO, CPO, and PG. They are defined as follows:

RO = Characteristic radius, ft;

VO = Characteristic velocity in gas phase, ft/sec;

TO = Characteristic temperature in gas phase, °R;

DENO = Characteristic density in gas phase, lb_m/cu.ft;

AMUO = Characteristic viscosity in gas phase, lb_m/ft/sec;

DO = Characteristic binary diffusion coefficient, sq. ft/sec;

WO = Characteristic species production rate, lb_m/cu.ft/sec;

ALAMO = Characteristic thermal conductivity in gas phase, Btu/hr/ft/°R;

CPO = Characteristic specific heat per unit mass at constant pressure, Btu/lb_m;

PG = Imposed favorable downstream pressure gradient, psf/ft

These 10 numbers are the characteristic values in the gas phase. The radius of the combustion chamber is normally chosen for RO. Values at the center of the combustion chamber are conveniently selected for VO, TO, DENO, AMUO, DO, ALAMO and CPO. For continued run, this input card should have the same values as that for the corresponding initial run.

4. The fourth input card consists of 10 numbers punched according to the format (10F8.0). These numbers are called by the following symbols: ANU1, ANU2, ANU3, TC, RA1, RA2, CE, SF, FLL and FLU. They are defined as follows:

   ANU1 = Stoicheiometric coefficient of oxidizer;

   ANU2 = Stoicheiometric coefficient of fuel;

   ANU3 = Stoicheiometric coefficient of product;

   TC = Minimum temperature for combustion to take place;

   RA1 = Molecular radius of oxidizer;

   RA2 = Molecular radius of fuel;

   CE = Activation energy, Kcal/g-mole;

   SF = Steric Factor;

   FLL = Lower flammability limit;

   FLU = Upper flammability limit.

   These are combustion data for chemical reaction of the form: Oxidizer + Fuel → Product. These numbers should not be changed for continued run.

5. The fifth input card consists of 6 numbers punched according to the format (6F8.0). These numbers are called by the following symbols: DENSO, TSO, ALAMSO, CSO, RRO and TSC. They are defined as follows:

   DENSO = Characteristic density in solid phase, lb_m/cu.ft;

   TSO = Characteristic temperature in solid phase, °R;

   ALAMSO = Characteristic thermal conductivity in solid phase, Btu/hr/ft/°R;

   CSO = Characteristic specific heat per unit mass in solid phase, Btu/lb_m/°R;

   RRO = Characteristic regression rate of solid surface, ft/sec;

   TSC = Minimum temperature for the fuel to vaporize, °R.

   The first five numbers are the characteristic values in the solid phase. This card should remain unchanged for continued run.

6. The number of input card that follows is NI. NI has a minimum value of 3. Each of these input cards consists of 8 numbers punched according to the format (3F10.0,E10.0,4F10.0). These numbers are called by the following symbols: AMI(I), CAI(I), CBI(I), CCI(I), HSL(I), HLG(I), HIO(I) and TBP (I), where I is 1 for the first card, 2 for the second card and NI for the last card. They are defined as follows:

   AMI(I) = Molecular weight of species I, lb_m/mole;

   CAI(I) = Constant, a_i, for the evaluation of C_{pi}, Btu/lb_m;

   CBI(I) = Constant, b_i, for the evaluation of C_{pi}, Btu/lb_m/°R;

   CCI(I) = Constant, c_i, for the evaluation of C_{pi}, Btu/lb_m/°R;

   HSL(I) = Heat of fusion of species I, Btu/lb_m;

   HLG(I) = Heat of vaporization of species I, Btu/lb_m;

HIO(I) = Heat of formation of species I, Btu/lb_m;

TBP(I) = Boiling point of species I, °R.

For the sake of consistency, the first, second and third of these NI cards should contain values corresponding to that of the oxidizer, the fuel and the product respectively. The values for any additional chemical species are then stored in the remaining input cards. These cards should stay the same for continued run.

7. For initial run, the initial values for the following dependent variables are read from card input:

   VR = Dimensionless radial velocity at all grid points in the gas phase at any time level, L, and the corresponding guess values at the next time level, L + 1;

   T = Dimensionless temperature at all grid points in the gas phase at any time level, L, and the corresponding guess values at the next time level, L + 1;

   TS = Dimensionless temperature at all grid points in the solid phase at any time level, L, and the corresponding guess values at the next time level, L + 1;

   YI1 = Mass fraction of NI chemical species at all grid points in the gas phase at any time level, L.

   Since the dimensionless radial velocity is usually relatively small in magnitude, it is convenient to express the dimensionless radial velocity at any grid point as a fraction of the corresponding value at the gas-solid interface. These scaled values are read in and the program reassigns the correct values for the radial velocity at all grid points. The storing sequence and format are as follows:

   READ(5,61) ((VR(1,M,N), N = 1, NZ), M = 1, NW)

   READ(5,61) ((T(1,M,N), N = 1, NZ), M = 1, NW)

```
READ(5,61) ((TS(1, MS,N) = 1, NZ), MS = 1, NWS)
READ(5,61) (((YI1(I,M,N), N = 1, NZ), M = 1, NW), I = 1, NI)
61 FORMAT(10F8.0)
```

where,

M is the radial grid number in the gas phase;

MS is the radial grid number in the solid phase;

N is the axial grid number.

For continued run, these input cards should be removed. Data stored on magnetic tape from the previous run are read in from tape 22. The arrangement of these input cards is best illustrated in the next article on sample input.

D. Sample Input

A listing of the sample input is shown as follows:

```
 20  15  10  10   8   3   3   3   7   1   1
 .005      .04          -12.      .01         .01        0.0        1.0E-30
 .25     20.0     3240.     .135  .00004  0.000296   1.0    .06        .3    .164
  1.5      2.0      1.0  3240.   3.433     1.43    50.0    1.0       0.5     3.5
 168.5    540.     122.     0.221  .0008   3240.
 32.0       .295        0.0         0.0        0.0      0.0        0.0      162.342
 26.98      0.26       0.0         0.0        170.      4710.      0.0       4932.27
101.96     0.27        0.0         0.0        510.      2590.    -7110.      6840.
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
.0       .0000009.0000009.0000009.0000009.0000009.0000009.0000009.0000009.0000009
.0       .0000071.0000071.0000071.0000071.0000071.0000071.0000071.0000071.0000071
.0       .000057 .000057 .000057 .000057 .000057 .000057 .000057 .000057 .000057
.0       .00045  .00045  .00045  .00045  .00045  .00045  .00045  .00045  .00045
.0       .00091  .00091  .00091  .00091  .00091  .00091  .00091  .00091  .00091
.0       .00183  .00183  .00183  .00183  .00183  .00183  .00183  .00183  .00183
.0       .0037   .0037   .0037   .0037   .0037   .0037   .0037   .0037   .0037
.0       .0074   .0074   .0074   .0074   .0074   .0074   .0074   .0074   .0074
.0       .015    .015    .015    .015    .015    .015    .015    .015    .015
.0       .03     .03     .03     .03     .03     .03     .03     .03     .03
.0       .061    .061    .061    .061    .061    .061    .061    .061    .061
.0       .123    .123    .123    .123    .123    .123    .123    .123    .123
.0       .25     .25     .25     .25     .25     .25     .25     .25     .25
.0       .5      .5      .5      .5      .5      .5      .5      .5      .5
 .0       .998    .998    .998    .998    .998    .998    .998    .998    .998
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
 1.0      1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0     1.0
```

D. Sample Input (continued)

```
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.      1.015    1.015    1.015    1.015    1.015    1.015    1.015    1.015    1.015
  1.       1.15     1.15     1.15     1.15     1.15     1.15     1.15     1.15     1.15
  1.       1.48     1.48     1.48     1.48     1.48     1.48     1.48     1.48     1.48
  1.      1.775    1.775    1.775    1.775    1.775    1.775    1.775    1.775    1.775
  1.       1.49     1.49     1.49     1.49     1.49     1.49     1.49     1.49     1.49
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  6.       6.       6.       6.       6.       6.       6.       6.       6.       6.
5.8215705.8215705.8215705.8215705.8215705.8215705.8215705.8215705.8215705.821570
5.6440265.6440265.6440265.6440265.6440265.6440265.6440265.6440265.6440265.644026
5.4673585.4673585.4673585.4673585.4673585.4673585.4673585.4673585.4673585.467358
5.2915595.2915595.2915595.2915595.2915595.2915595.2915595.2915595.2915595.291559
5.1166195.1166195.1166195.1166195.1166195.1166195.1166195.1166195.1166195.116619
4.9425304.9425304.9425304.9425304.9425304.9425304.9425304.9425304.9425304.942530
4.4252914.4252914.4252914.4252914.4252914.4252914.4252914.4252914.4252914.425291
3.9154233.9154233.9154233.9154233.9154233.9154233.9154233.9154233.9154233.915423
3.4127203.4127203.4127203.4127203.4127203.4127203.4127203.4127203.4127203.412720
2.9169832.9169832.9169832.9169832.9169832.9169832.9169832.9169832.9169832.916983
2.4280212.4280212.4280212.4280212.4280212.4280212.4280212.4280212.4280212.428021
1.9456531.9456531.9456531.9456531.9456531.9456531.9456531.9456531.9456531.945653
1.4697021.4697021.4697021.4697021.4697021.4697021.4697021.4697021.4697021.469702
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
  1.       .97      .97      .97      .97      .97      .97      .97      .97      .97
  1.       .84      .84      .84      .84      .84      .84      .84      .84      .84
  1.       .63      .63      .63      .63      .63      .63      .63      .63      .63
  1.       .33      .33      .33      .33      .33      .33      .33      .33      .33
  1.       0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
```

D. Sample Input (continued)

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
.0	.03	.03	.03	.03	.03	.03	.03	.03	.03
.0	.16	.16	.16	.16	.16	.16	.16	.16	.16
.0	.37	.37	.37	.37	.37	.37	.37	.37	.37
.0	.67	.67	.67	.67	.67	.67	.67	.67	.67
.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

E. Output of Program HETCOMB

The output of program HETCOMB consists of printed output, punched card output and magnetic tape output. The punched card output can be saved and later rearranged as input for program PLOT. The magnetic tape output should be saved as input for the next continued run. The sequence of the printed output is as follows:

1. The input values for the following symbols are printed first: NW, NWS, NZ, NT, N, NT, NR, NRS, NX, NXS, DELR, DELRS, DELZ, DELT, AE, AMIN, AMAX. The characteristic values and constant in the solid phase, DENSO, TSO, ALAMSO, CSO, RRO and TSC, are then printed.
2. The characteristic values and constants in the gas phase, RO, VO, TO, DENO, AMUO, DO, WO, ALAMO, CPO, PG, AMI(I), CAI(I), CBI(I), CCI(I), HSL(I), HLG(I), HIO(I) and TBP(I), are printed first on the second page. Then, the combustion data, ANU1, ANU2, ANU3, SF, FLL, FLU, RA1, RA2 and CE, are printed.
3. On the third page, the dimensionless group, RE, SC, PR, EC, DAM, DFURS1, DFURA2, DFURA3, DFURA4, DFURA5, DENRA, VRA, TRA and ALAMRA are defined and their calculated values are printed.
4. The variables, DEN, VR, VZ, T, TS, YI1, P, AMU, ALAM, CP, DI1, WI1, CPI1, CI1, DENS, ALAMS, CR, RR and HSGI at time step, L = 1, are converted to their appropriate dimension units and printed in the form of tables.
5. Values for the dependent variables, DEN, VR, TZ, T, TS and YI1, at every other LL time step are printed in the appropriate dimension units in the form of tables. In each of these tables, the time step

number, L, the number of iterations taken, IT, and the total time elapsed, TIME, are also specified.

6. There are two possible ways for this program to terminate. Hence, there are two possible terminate print outs as follows:

   (a) If the convergence criteria are not met at end of NIT iterations during any time step, the program terminates with the statement, "TERMINATE PROGRAM AT END OF NIT ITERATIONS" and values for K, M, N, MS and AD are printed out.

   (b) If the specified job is completed, the program terminates with the statement, "TERMINATE PROGRAM AT END OF NT TIME STEPS".

F. Sample Printed Output

```
                                        INPUT DATA
                                        ----------

NUMBER OF GRID USED=          NW =  20        NWS =  15        NZ =  10

NUMBER OF TIME STEPS, NT =    1     NUMBER OF SPECIES, NI =   3     ITERATIONS ALLOWED, NIT =   7

GRID POSITIONS AT WHICH RADIAL GRID SIZES ARE CHANGED =          NR =  10        NRS =   8

RATIO OF RADIAL GRID SIZES FOR NON-UNIFORM RADIAL GRID =         NX =   3        NXS =   3

GRID SIZES=          DELR =  .026571        DELRS =  .005000        DELZ =  .040000

SIZE OF TIME STEP, DELT =    2.441E-04                    ALLOWED ERROR, AE =  .010000

MINIMUM ALLOWED ABSOLUTE VALUE, AMIN =    1.000E-30
MAXIMUM ALLOWED DIFFERENCE, AMAX =     .0100

CHARACTERISTIC VALUES AND CONSTANTS IN SOLID PHASE
--------------------------------------------------

DENSO  =  163.50     LBM/FT/FT/FT                    TSO =   540.0     DEGREE R

ALAMSO =  122.00     BTU/HR/FT/DEGREE R              CSO =   .2210     BTU/LBM/DEGREE R

RRO    =   9.000E-04 FT/SEC                          TSC =  3240.0     DEGREE R
```

CHARACTERISTIC VALUES AND CONSTANTS IN GAS PHASE

RO	=	.250000 FT	VO	=	20.0000 FT/SEC
TO	=	3240.00 DEGREE R	DENO	=	.135000 LBM/FT/FT/FT
AMUO	=	.000040 LBM/SEC/FT	DO	=	.000296 FT*FT/SEC
WO	=	1.000000 LBM/FT/FT/FT/SEC	ALAMO	=	.060000 BTU/HR/FT/DEGREE R
CPO	=	.300000 BTU/LBM/DEGREE R	PG	=	.164000 PSF./FT.

SPECIES 1 =	AMI =	32.00	CAI =	.29500	HSL =	0.	BTU/LBM	HLG =	0.	BTU/LBM
	CBI =	0.	CCI =	0.	HIO =	0.	BTU/LBM	TBP =	162.34	DEGREE R
SPECIES 2 =	AMI =	26.99	CAI =	.26000	HSL =	170.00	BTU/LBM	HLG =	4710.0	BTU/LBM
	CBI =	0.	CCI =	0.	HIO =	0.	BTU/LBM	TBP =	4932.3	DEGREE R
SPECIES 3 =	AMI =	102.0	CAI =	.27000	HSL =	510.00	BTU/LBM	HLG =	2590.0	BTU/LBM
	CBI =	0.	CCI =	0.	HIO =	-7110.0	BTU/LBM	TBP =	6840.0	DEGREE R

COMBUSTION DATA

ANU1 = 1.50 ANU2 = 2.00 ANU3 = 1.00

SF = 1.000 FLL = .500 FLU = 3.500 TC = 3240.00 DEGREE R

RA1 = 3.4330 ANGSTROM RA2 = 1.4300 ANGSTROM CF = 50.000 KCAL/G-MOLE

CALCULATED CONSTANTS

VALUES OF DIMENSIONLESS GROUPS

$$RE = \frac{DEN0*V0*R0}{AMU0} = 1.6875E+04$$

$$SC = \frac{AMU0}{DEN0*D0} = 1.001$$

$$PR = \frac{CP0*AMU0}{ALAM0} = .7200$$

$$EC = \frac{V0*V0}{CP0*T0} = 1.6436E-05$$

$$DA1 = \frac{R0*W0}{DEN0*V0} = 5.2593E-02$$

$$DEURA1 = \frac{D0}{R0*V0} = 5.9200E-05$$

$$DEURA2 = \frac{D0}{ALPHA0} = .7193$$

$$DEURA3 = \frac{R0*V0}{ALPHA0} = 1.2150E+04$$

$$DEURA4 = \frac{R0*V0}{ALPHAS0} = 5494$$

$$DEURA5 = \frac{R0*RR0}{ALPHAS0} = .2198$$

$$DENRA = \frac{DENS0}{DEN0} = 1248$$

$$VRA = \frac{RR0}{V0} = 4.0000E-05$$

$$TRA = \frac{TS0}{T0} = .1667$$

$$ALAMRA = \frac{ALAMS0}{ALAM0} = 2033$$

INPUT= TIME STEP = 1

TIME = 0. SEC.

DENSITY AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
2	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
3	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
4	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
5	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
6	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
7	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
8	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
9	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
10	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
11	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
12	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
13	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
14	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
15	.13500	.13300	.13300	.13300	.13300	.13300	.13300	.13300	.13300	.13300
16	.13500	.11674	.11674	.11674	.11674	.11674	.11674	.11674	.11674	.11674
17	.13500	8.85792E-02	8.85792E-02	8.85792E-02	8.85792E-02	8.85792E-02	8.85792E-02	8.85791E-02	8.85791E-02	8.85791E-02
18	.13500	7.11576E-02	7.11576E-02	7.11576E-02	7.11576E-02	7.11576E-02	7.11576E-02	7.11576E-02	7.11575E-02	7.11575E-02
19	.13500	8.05611E-02	8.05611E-02	8.05610E-02	8.05610E-02	8.05610E-02	8.05610E-02	8.05610E-02	8.05610E-02	8.05610E-02
20	.13500	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382

INPUT= TIME STEP = 1 TIME = 0. SEC.

R-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	-8.19722E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07	-8.19723E-07
7	0.	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06	-6.46670E-06
8	0.	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05	-5.19158E-05
9	0.	-4.09861E-04	-4.09861E-04	-4.09861E-04	-4.09861E-04	-4.09861E-04	-4.09861E-04	-4.09861E-04	-4.09862E-04	-4.09862E-04
10	0.	-8.28830E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04	-8.28831E-04
11	0.	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03	-1.66677E-03
12	0.	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03	-3.36997E-03
13	0.	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73994E-03	-6.73995E-03
14	0.	-1.36620E-02	-1.36620E-02	-1.36620E-02	-1.36620E-02	-1.36620E-02	-1.36620E-02	-1.36620E-02	-1.36621E-02	-1.36621E-02
15	0.	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02	-2.73241E-02
16	0.	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02	-5.55590E-02
17	0.	-.11203	-.11203	-.11203	-.11203	-.11203	-.11203	-.11203	-.11203	-.11203
18	0.	-.22770	-.22770	-.22770	-.22770	-.22770	-.22770	-.22770	-.22770	-.22770
19	0.	-.45540	-.45540	-.45540	-.45540	-.45540	-.45540	-.45540	-.45540	-.45540
20	0.	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080

INPUT= TIME STEP = 1

TIME = 0. SEC.

Z-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000
2	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746
3	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470
4	19.168	19.168	19.168	19.168	19.168	19.168	19.168	19.168	19.168	19.168
5	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836
6	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463
7	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040
8	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546
9	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952
10	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723
11	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473
12	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198
13	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892
14	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546
15	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146
16	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671
17	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080
18	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288
19	12.035	12.035	12.035	12.035	12.035	12.035	12.035	12.035	12.035	12.035
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

INPUT= TIME STEP = 1

TIME = 0. SEC.

GAS PHASE TEMPERATURE AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
3	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
4	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
5	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
6	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
7	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
8	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
9	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
10	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
11	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
12	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
13	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
14	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
15	3240.0	3288.6	3288.6	3288.6	3288.6	3288.6	3288.6	3288.6	3288.6	3288.6
16	3240.0	3726.0	3726.0	3726.0	3726.0	3726.0	3726.0	3726.0	3726.0	3726.0
17	3240.0	4795.2	4795.2	4795.2	4795.2	4795.2	4795.2	4795.2	4795.2	4795.2
18	3240.0	5751.0	5751.0	5751.0	5751.0	5751.0	5751.0	5751.0	5751.0	5751.0
19	3240.0	4827.6	4827.6	4827.6	4827.6	4827.6	4827.6	4827.6	4827.6	4827.6
20	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0

INPUT= TIME STEP = 1

TIME = 0. SEC.

TEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6
3	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8
4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4
5	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4
6	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0
7	2669.0	2669.0	2669.0	2669.0	2669.0	2669.0	2669.0	2669.0	2669.0	2669.0
8	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7
9	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3
10	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9
11	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2
12	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1
13	1050.7	1050.7	1050.7	1050.7	1050.7	1050.7	1050.7	1050.7	1050.7	1050.7
14	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64
15	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

INPUT= TIME STEP = 1

TIME = 0. SEC.

MASS FRACTION OF SPECIES. 1. AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
4	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
5	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
6	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
7	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
8	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
9	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
10	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
11	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
12	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
13	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
14	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
15	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
16	1.0000	.97000	.97000	.97000	.97000	.97000	.97000	.97000	.97000	.97000
17	1.0000	.84000	.84000	.84000	.84000	.84000	.84000	.84000	.84000	.84000
18	1.0000	.63000	.63000	.63000	.63000	.63000	.63000	.63000	.63000	.63000
19	1.0000	.33000	.33000	.33000	.33000	.33000	.33000	.33000	.33000	.33000
20	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.

INPUT= TIME STEP = 1 TIME = 0. SEC.

MASS FRACTION OF SPECIES, 2, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02	3.00000E-02
17	0.	.16000	.16000	.16000	.16000	.16000	.16000	.16000	.16000	.16000
18	0.	.37000	.37000	.37000	.37000	.37000	.37000	.37000	.37000	.37000
19	0.	.67000	.67000	.67000	.67000	.67000	.67000	.67000	.67000	.67000
20	0.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

INPUT= TIME STEP = 1

TIME = 0. SEC.

MASS FRACTION OF SPECIES, 3, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
19	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT L = 1

TIME = 0. SEC.

PRESSURE AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
2	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
3	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
4	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
5	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
6	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
7	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
8	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
9	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
10	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
11	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
12	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
13	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
14	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
15	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
16	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
17	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
18	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
19	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
20	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

VISCOSITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
2	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
3	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
4	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
5	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
6	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
7	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
8	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
9	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
10	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
11	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
12	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
13	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
14	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
15	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
16	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
17	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
18	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
19	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04
20	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

THERMAL CONDUCTIVITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
2	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
3	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
4	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
5	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
6	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
7	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
8	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
9	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
10	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
11	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
12	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
13	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
14	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
15	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
16	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
17	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
18	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
19	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000
20	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000	1.2000

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

SPECIFIC HEAT AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
2	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
3	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
4	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
5	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
6	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
7	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
8	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
9	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
10	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
11	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
12	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
13	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
14	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
15	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
16	.29500	.29395	.29395	.29395	.29395	.29395	.29395	.29395	.29395	.29395
17	.29500	.28940	.28940	.28940	.28940	.28940	.28940	.28940	.28940	.28940
18	.29500	.28205	.28205	.28205	.28205	.28205	.28205	.28205	.28205	.28205
19	.29500	.27155	.27155	.27155	.27155	.27155	.27155	.27155	.27155	.27155
20	.29500	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

DIFFUSION COEFFICIENT OF SPECIES. 1. AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
2	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
3	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
4	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
5	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
6	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
7	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
8	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
9	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
10	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
11	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
12	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
13	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
14	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
15	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
16	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
17	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
18	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
19	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
20	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

RATE OF PRODUCTION OF SPECIES. 1. AT GRID POINT(M.N)

N= M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.	-6.0022	-6.0022	-6.0022	-6.0022	-6.0022	-6.0022	-6.0022	-6.0022	-6.0022
19	0.	-3.0387	-3.0387	-3.0387	-3.0387	-3.0387	-3.0387	-3.0387	-3.0387	-3.0387
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

SPECIFIC HEAT PER UNIT MASS OF SPECIES. 1. AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
2	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
3	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
4	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
5	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
6	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
7	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
8	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
9	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
10	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
11	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
12	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
13	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
14	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
15	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
16	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
17	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
18	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
19	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500
20	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500	.29500

CALCULATED VALUES AT I = 1 TIME = 0. SEC.

ENTHALPY PER UNIT MASS OF SPECIES. 1. AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
2	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
3	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
4	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
5	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
6	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
7	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
8	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
9	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
10	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
11	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
12	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
13	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
14	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56
15	797.56	811.90	811.90	811.90	811.90	811.90	811.90	811.90	811.90	811.90
16	797.56	940.93	940.93	940.93	940.93	940.93	940.93	940.93	940.93	940.93
17	797.56	1256.3	1256.3	1256.3	1256.3	1256.3	1256.3	1256.3	1256.3	1256.3
18	797.56	1538.3	1538.3	1538.3	1538.3	1538.3	1538.3	1538.3	1538.3	1538.3
19	797.56	1265.9	1265.9	1265.9	1265.9	1265.9	1265.9	1265.9	1265.9	1265.9
20	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56	797.56

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

DIFFUSION COEFFICIENT OF SPECIES, 2, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
2	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
3	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
4	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
5	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
6	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
7	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
8	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
9	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
10	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
11	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
12	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
13	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
14	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
15	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
16	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
17	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
18	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
19	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
20	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

RATE OF PRODUCTION OF SPECIES, 2, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.	-6.7475	-6.7475	-6.7475	-6.7475	-6.7475	-6.7475	-6.7475	-6.7475	-6.7475
19	0.	-3.4160	-3.4160	-3.4160	-3.4160	-3.4160	-3.4160	-3.4160	-3.4160	-3.4160
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

SPECIFIC HEAT PER UNIT MASS OF SPECIES, 2. AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
2	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
3	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
4	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
5	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
6	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
7	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
8	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
9	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
10	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
11	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
12	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
13	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
14	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
15	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
16	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
17	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
18	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
19	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000
20	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000	.26000

CALCULATED VALUES AT I = 1 TIME = 0. SEC.

ENTHALPY PER UNIT MASS OF SPECIES. 2, AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
2	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
3	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
4	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
5	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
6	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
7	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
8	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
9	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
10	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
11	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
12	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
13	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
14	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94
15	872.94	885.57	885.57	885.57	885.57	885.57	885.57	885.57	885.57	885.57
16	872.94	999.30	999.30	999.30	999.30	999.30	999.30	999.30	999.30	999.30
17	872.94	1277.3	1277.3	1277.3	1277.3	1277.3	1277.3	1277.3	1277.3	1277.3
18	872.94	6235.8	6235.8	6235.8	6235.8	6235.8	6235.8	6235.8	6235.8	6235.8
19	872.94	1285.7	1285.7	1285.7	1285.7	1285.7	1285.7	1285.7	1285.7	1285.7
20	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94	872.94

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

DIFFUSION COEFFICIENT OF SPECIES, 3, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
2	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
3	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
4	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
5	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
6	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
7	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
8	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
9	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
10	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
11	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
12	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
13	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
14	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
15	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
16	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
17	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
18	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
19	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03
20	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03	5.92000E-03

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

RATE OF PRODUCTION OF SPECIES, 3, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.	12.750	12.750	12.750	12.750	12.750	12.750	12.750	12.750	12.750
19	0.	6.4547	6.4547	6.4547	6.4547	6.4547	6.4547	6.4547	6.4547	6.4547
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

SPECIFIC HEAT PER UNIT MASS OF SPECIES, 3, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
2	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
3	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
4	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
5	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
6	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
7	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
8	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
9	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
10	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
11	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
12	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
13	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
14	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
15	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
16	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
17	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
18	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
19	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000
20	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000	.27000

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

ENTHALPY PER UNIT MASS OF SPECIES. 3. AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
2	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
3	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
4	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
5	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
6	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
7	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
8	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
9	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
10	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
11	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
12	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
13	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
14	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0
15	-5870.0	-5856.9	-5856.9	-5856.9	-5856.9	-5856.9	-5856.9	-5856.9	-5856.9	-5856.9
16	-5870.0	-5738.8	-5738.8	-5738.8	-5738.8	-5738.8	-5738.8	-5738.8	-5738.8	-5738.8
17	-5870.0	-5450.1	-5450.1	-5450.1	-5450.1	-5450.1	-5450.1	-5450.1	-5450.1	-5450.1
18	-5870.0	-5192.1	-5192.1	-5192.1	-5192.1	-5192.1	-5192.1	-5192.1	-5192.1	-5192.1
19	-5870.0	-5441.4	-5441.4	-5441.4	-5441.4	-5441.4	-5441.4	-5441.4	-5441.4	-5441.4
20	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0	-5870.0

CALCULATED VALUES AT L = 1

TIME = 0. SEC.

DENSITY OF SOLID FUEL AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
2	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
3	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
4	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
5	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
6	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
7	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
8	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
9	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
10	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
11	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
12	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
13	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
14	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50
15	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50	168.50

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

CALCULATED VALUES AT L = 1 TIME = 0. SEC.

THERMAL CONDUCTIVITY OF SOLID FUEL AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
2	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
3	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
4	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
5	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
6	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
7	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
8	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
9	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
10	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
11	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
12	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
13	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
14	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00
15	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00	122.00

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

CALCULATED VALUES AT I 1 TIME = 0. SEC.

SPECIFIC HEAT PER UNIT MASS OF SOLID FUEL AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
2	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
3	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
4	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
5	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
6	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
7	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
8	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
9	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
10	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
11	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
12	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
13	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
14	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100
15	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100	.22100

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

CALCULATED VALUES AT I = 1 TIME = 0. SEC.

REGRESSION RATE OF FUEL AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	0.	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04	8.00000E-04

HEAT OF SUBLIMATION OF SPECIES. 1. AT GRID POINT(M,N)

1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

HEAT OF SUBLIMATION OF SPECIES. 2. AT GRID POINT(M,N)

1	4880.0	4880.0	4880.0	4880.0	4880.0	4880.0	4880.0	4880.0	4880.0	4880.0

HEAT OF SUBLIMATION OF SPECIES. 3. AT GRID POINT(M,N)

1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

NOTE MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

TIME = 3.0518E-06 SEC.

DENSITY AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	.13500	.13499	.13499	.13499	.13499	.13499	.13499	.13499	.13499	.13499
2	.13500	.13499	.13499	.13499	.13499	.13499	.13499	.13499	.13499	.13499
3	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
4	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
5	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
6	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
7	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
8	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
9	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
10	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
11	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
12	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
13	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
14	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500	.13500
15	.13500	.13300	.13300	.13300	.13300	.13300	.13300	.13300	.13300	.13300
16	.13500	.11676	.11673	.11673	.11673	.11673	.11673	.11673	.11673	.11673
17	.13500	8.85459E-02	8.85722E-02	8.85736E-02	8.85738E-02	8.85738E-02	8.85738E-02	8.85738E-02	8.85738E-02	8.85737E-02
18	.13500	7.12331E-02	7.11070E-02	7.11102E-02	7.11106E-02	7.11106E-02	7.11106E-02	7.11106E-02	7.11106E-02	7.11106E-02
19	.13500	8.06468E-02	8.04503E-02	8.04614E-02	8.04622E-02	8.04622E-02	8.04622E-02	8.04622E-02	8.04621E-02	8.04621E-02
20	.13500	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382

CALCULATED VALUES AT L = 2. IT = 3 TIME = 3.0518E-06 SEC.

R-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	2.95567E-11	1.05560E-11	-1.11830E-23	1.01714E-19	2.94806E-19	3.02935E-18	3.00425E-18	2.93139E-18	3.38391E-18
3	0.	1.20333E-11	-1.15754E-12	-7.26183E-25	6.61915E-21	2.18837E-18	2.67095E-18	2.28007E-18	2.24003E-18	1.71777E-18
4	0.	1.02197E-11	-1.40605E-14	-6.03159E-23	5.08438E-19	3.93506E-18	4.03448E-18	3.93492E-18	4.02065E-18	3.97937E-18
5	0.	5.41337E-12	-8.69709E-12	-7.41150E-12	-7.58060E-12	-7.58058E-12	-7.58059E-12	-7.58059E-12	-7.58059E-12	-7.58059E-12
6	0.	-8.18913E-07	-8.19756E-07	-8.19774E-07	-8.19777E-07	-8.19777E-07	-8.19777E-07	-8.19777E-07	-8.19777E-07	-8.19777E-07
7	0.	-6.45963E-06	-6.46696E-06	-6.46709E-06	-6.46712E-06	-6.46712E-06	-6.46712E-06	-6.46713E-06	-6.46713E-06	-6.46713E-06
8	0.	-5.18605E-05	-5.19178E-05	-5.19188E-05	-5.19191E-05	-5.19191E-05	-5.19191E-05	-5.19191E-05	-5.19191E-05	-5.19191E-05
9	0.	-4.09427E-04	-4.09854E-04	-4.09866E-04	-4.09865E-04	-4.09865E-04	-4.09865E-04	-4.09865E-04	-4.09865E-04	-4.09865E-04
10	0.	-8.27709E-04	-8.28842E-04	-8.28854E-04	-8.28872E-04	-8.28872E-04	-8.28872E-04	-8.28872E-04	-8.28872E-04	-8.28873E-04
11	0.	-1.66455E-03	-1.66682E-03	-1.66680E-03	-1.66688E-03	-1.66688E-03	-1.66688E-03	-1.66688E-03	-1.66688E-03	-1.66688E-03
12	0.	-3.36557E-03	-3.37007E-03	-3.36981E-03	-3.37019E-03	-3.37019E-03	-3.37019E-03	-3.37019E-03	-3.37019E-03	-3.37019E-03
13	0.	-6.73127E-03	-6.74015E-03	-6.73996E-03	-6.74039E-03	-6.74039E-03	-6.74039E-03	-6.74039E-03	-6.74039E-03	-6.74039E-03
14	0.	-1.35449E-02	-1.36624E-02	-1.36620E-02	-1.36629E-02	-1.36629E-02	-1.36629E-02	-1.36629E-02	-1.36629E-02	-1.36629E-02
15	0.	-2.72905E-02	-2.73250E-02	-2.73248E-02	-2.73260E-02	-2.73260E-02	-2.73260E-02	-2.73260E-02	-2.73260E-02	-2.73260E-02
16	0.	-5.54930E-02	-5.55611E-02	-5.55616E-02	-5.55631E-02	-5.55631E-02	-5.55631E-02	-5.55631E-02	-5.55631E-02	-5.55631E-02
17	0.	-.11130	-.11203	-.11204	-.11204	-.11204	-.11204	-.11204	-.11204	-.11204
18	0.	-.22745	-.22772	-.22773	-.22773	-.22773	-.22773	-.22773	-.22773	-.22773
19	0.	-.45494	-.45544	-.45546	-.45546	-.45546	-.45546	-.45546	-.45546	-.45546
20	0.	-.91081	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080	-.91080

CALCULATED VALUES AT L = 2, IT = 3 TIME = 3.0518E-06 SEC.

Z-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000
2	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746	19.746
3	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470	19.470
4	19.169	19.169	19.169	19.169	19.169	19.169	19.169	19.169	19.169	19.169
5	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836	18.836
6	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463	18.463
7	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040	18.040
8	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546	17.546
9	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952	16.952
10	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723	16.723
11	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473	16.473
12	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198	16.198
13	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892	15.892
14	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546	15.546
15	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146	15.146
16	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671	14.671
17	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080	14.080
18	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288	13.288
19	12.035	12.034	12.034	12.034	12.034	12.034	12.034	12.034	12.034	12.034
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT L = 2, TT = 3

TIME = 3.0518E-06 SEC.

GAS PHASE TEMPERATURE AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1
2	3240.0	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1	3240.1
3	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
4	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
5	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
6	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
7	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
8	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
9	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
10	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
11	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
12	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
13	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
14	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
15	3240.0	3288.6	3288.7	3288.7	3288.7	3288.7	3288.7	3288.7	3288.7	3288.7
16	3240.0	3725.6	3726.1	3726.1	3726.2	3726.2	3726.2	3726.2	3726.2	3726.2
17	3240.0	4793.6	4795.3	4795.3	4795.4	4795.4	4795.4	4795.4	4795.4	4795.4
18	3240.0	5748.6	5753.0	5753.2	5753.2	5753.2	5753.2	5753.2	5753.2	5753.2
19	3240.0	4825.8	4831.0	4831.1	4831.1	4831.1	4831.1	4831.1	4831.1	4831.1
20	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0

CALCULATED VALUES AT L = 2. IT = 3 TIME = 3.0518E-06 SEC.

TEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6	3143.6
3	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8	3047.8
4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4	2952.4
5	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4	2857.4
6	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0	2763.0
7	2668.9	2668.9	2668.9	2668.9	2668.9	2668.9	2668.9	2668.9	2668.9	2668.9
8	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7	2389.7
9	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3	2114.3
10	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9	1842.9
11	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2	1575.2
12	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1	1311.1
13	1050.7	1050.6	1050.6	1050.6	1050.6	1050.6	1050.6	1050.6	1050.6	1050.6
14	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64	793.64
15	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00

NOTE MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

CALCULATED VALUES AT L = 2, IT = 3 TIME = 3.0518E-06 SEC.

MASS FRACTION OF SPECIES, 1, AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
2	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
3	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
4	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
5	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
10	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
11	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
13	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.0000	1.0000
14	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
15	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
16	1.0000	.97002	.96999	.96999	.96999	.96999	.96999	.96999	.96999	.96999
17	1.0000	.84015	.83999	.83999	.83999	.83999	.83999	.83999	.83999	.83999
18	1.0000	.63039	.62996	.62995	.62995	.62995	.62995	.62995	.62995	.62995
19	1.0000	.33071	.32993	.32992	.32991	.32991	.32991	.32991	.32991	.32991
20	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.

CALCULATED VALUES AT I = 2, TT = 3 TIME = 3.0518E-06 SEC.

MASS FRACTION OF SPECIES, 3, AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.	3.20014E-05	8.60179E-05	8.58114E-05	8.59264E-05	8.59260E-05	8.59260E-05	8.59260E-05	8.59260E-05	8.59260E-05
19	0.	4.90310E-05	1.35907E-04	1.34355E-04	1.35098E-04	1.35097E-04	1.35097E-04	1.35097E-04	1.35097E-04	1.35097E-04
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

NOTE M IS GRID NUMBER IN RADIAL DIRECTION
N IS GRID NUMBER IN AXIAL DIRECTION

TERMINATE PROGRAM AT END OF 1 TIME STEPS.

G. Storage Requirement and Time Limit

The storage requirement for this computer program depends primarily on the dimensions specified for the dimensioned variables in the DIMENSION and COMMON statements. For the particular case as shown in Section B-H, where the maximum values for NW, NWS, NZ and NI are 20, 15, 10 and 3 respectively, the storage requirement for both compilation and execution is 120K(octal). If all the dimensions specified as 20 in the DIMENSION and COMMON statements are replaced by a value equal to 40, i.e., a maximum value of 40 is allowed for NW, the storage requirement is 150K(octal). If all the dimensions specified as 10 in the DIMENSION and COMMON statements are replaced by a value equal to 20, i.e., a maximum value of 20 is allowed for NZ, the storage requirement is 160K(octal).

The calculation time required per time step depends mainly on the number of iterations necessary for convergence in a time step. This, in turn, depends on the value specified for the time increment, DELT, and the convergence criteria used, namely, values for AE and AMAX. In general, more iterations are required at the start of the transient calculation and as the solution tends towards the steady state conditions, fewer iterations are necessary. For the particular case as specified in Section B.B, the actual running time per 1000 time steps varies from 20 to 40 minutes corresponding to 2 to 4 iterations per time step. The total time necessary for the transient solution to reach the steady state conditions is approximately twice the time required for the oxidizer at the inlet to reach the exit. For the particular case as specified in Section B.B, a total of 3000 time steps are necessary to reach the steady state

conditions and approximately $1\frac{1}{2}$ hours of actual running time on the CDC6600 computer are required.

H. Program Listing

```
C-----
      PROGRAM HETCOMB(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8,TAPE22
     1,PUNCH)
C-----
C     THIS PROGRAM IS TO PERFORM A THEORETICAL STUDY OF HETEROGENEOUS
C     COMBUSTION.
C     THE INDEPENDENT VARIABLES ARE THE RADIAL DISTANCE, THE AXIAL
C     DISTANCE AND TIME.
C     THIS PROGRAM CALCULATES THE DEPENDENT VARIABLES, DENSITY, RADIAL
C     VELOCITY, AXIAL VELOCITY, TEMPERATURE AND MASS FRACTION OF SPECIES
C     , I, IN THE GAS PHASE AND TEMPERATURE IN THE SOLID PHASE.
C-----
000003      DIMENSION YI1(3,20,10),YI2(3,20,10),DELTYB(3,20,10),TEMY(3,20,10),
     1TEMT(20,10),TEMS(15,10),TEMR(20,10),TEMZ(20,10),DELTTA(20,10),
     2DELTTB(20,10),DELTSA(15,10),DELTSB(15,10),DELTRA(20,10),
     3DELTRB(20,10),DELTZA(20,10),DELTZB(20,10),DELTYA(3,20,10)
C-----
000003      COMMON PO,AMUO,CO,WO,ALAMO,CPO,DENSO,ALAMSO,CSO,ERO,EC,
     1AMI(3),CAI(3),CBI(3),CCI(3),HSI(3),HIO(3),CP(2,20,10),HLG(3),
     2F(2,20,10), AMU(2,20,10), ALAM(2,20,10), HSGI(2,20,10),TBP(3),
     3DENS(2,15,10), CS(2,15,10), RR(2,10), ALAMS(2,15,10)
C-----
000003      COMMON/CAL/VR(2,20,10),VZ(2,20,10),TEMPR(20,10),TEMPZ(20,10),
     1TEMPT(20,10),TEMPS(15,10),TEMPY(3,20,10)
C-----
000003      COMMON/ECRM/NW,NWS,NZ,NI,ANU1,ANU2,ANU3,CF,TC,TSC,FLI,FLU,L,IT,SF,
     1RA1,RA2,VO,TC,DENO,TSO,TIME,DEN(2,20,10),T(2,20,10),TS(2,15,10)
C-----
000003      COMMON/FUN/DELR,DELZ,R(20)
C-----
000003      COMMON/SPEC/DI1(3,20,10),DI2(3,20,10),WI1(3,20,10),WI2(3,20,10),
     1CPI1(3,20,10),CPI2(3,20,10),HI1(3,20,10),HI2(3,20,10)
C-----
C     STORE NUMBER OF GRID USED.
C     DEFINE THE AVAILABLE OPTIONS FOR THE RADIAL GRID SIZES.
C     STORE NUMBER OF SPECIES PRESENT, NUMBER OF ITERATIONS ALLOWED,
C     NUMBER OF TIME STEPS, NUMBER OF STEPS BEFORE CALCULATED VALUES
C     ARE PRINTED OUT.
C     NOTE = FOR NON-UNIFORM RADIAL GRID SIZES, NR AND NRS SHOULD BE
C     SMALLER THAN NW AND NWS RESPECTIVELY.
C-----
000003      READ(5,11) NW , NWS, NZ, NR, NRS, NX, NXS, NI, NIT, NT, II
```

```
000035      11 FORMAT(11I4)                                                   4300000
000035         WRITE (6,12) NW, NWS,NZ,NT,NI,NIT,NR,NRS,NX,NXS                4400000
000065      12 FORMAT(1H1//50X,10HINPUT DATA,/50X,10H---------- ///2X,21HNUMBER O  4500000
           1F GRID USED= ,9X,5HNW = ,I3,9X,6HNWS = ,I3,9X,5HNZ = ,I3///2X,     4600000
           227HNUMBER OF TIME STEPS, NT = ,I4,5X,24HNUMBER OF SPECIES, NI = ,  4700000
           3I3,5X,26HITERATIONS ALLOWED, NIT = , I3///2X,56HGRID POSITIONS AT  4800000
           4WHICH RADIAL GRID SIZES ARE CHANGED = ,9X,5HNR = I3,9X,6HNRS = I3  4900000
           5///2X,57HRATIO OF RADIAL GRID SIZES FOR NON-UNIFORM RADIAL GRID =  5000000
           6,9X,5HNX = ,I3,9X,6HNXS = ,I3)                                    5100000
      C-----                                                                  5200000
      C     SET UPPER LIMITS FOR CERTAIN DO LOOPS.                            5300000
      C-----                                                                  5400000
000065        NW1 = NW - 1                                                    5500000
000067        NWS1 = NWS - 1                                                  5600000
000071        NZ1 = NZ - 1                                                    5700000
000072        NZ2 = NZ - 2                                                    5800000
000074        NI1 = NI - 1                                                    5900000
000075        NT1 = NT + 1                                                    6000000
      C-----                                                                  6100000
      C     STORE GRID SIZES, SIZE OF TIME STEP, CONVERGENCE CRITIERA AND     6200000
      C     AN ALLOWED MINIMUM ABSOLUTE VALUE.                                6300000
      C     NOTE = FOR INITIAL CALCULATION, SET TIME = ZERO.                  6400000
      C     OTHERWISE, SET ANY VALUE OTHER THAN ZERO FOR TIME.                6500000
      C-----                                                                  6600000
000077        IF(NW-NR) 15, 15, 18                                            6700000
000101      15 DELR = 1.0/(NW-1)                                              6800000
000105         GO TO 20                                                       6900000
000106      18 DELR = 1.0/(NW-NR+1+NX*(NR-2))                                 7000000
000116      20 READ(5,21) DELRS, DELZ, DELT, AE, AMAX, TIME, AMIN             7100000
000140      21 FORMAT(6F10.0,F10.0 )                                          7200000
000140         DELT = 2.0**DELT                                               7300000
000144         FT = 0.25/DELT                                                 7400000
000146         WRITE (6,22) DELR, DELRS, DELZ, DELT, AE, AMIN,AMAX            7500000
000167      22 FORMAT(///2X,12HGRID SIZES= ,9X,7HDELR = ,F8.6,9X,8HDELRS = ,F8.6,  7600000
           1 9X,7HDELZ = ,F8.6///2X,25HSIZE OF TIME STEP, DELT = ,F12.3,20X,   7700000
           220HALLOWED ERROR, AE = ,F8.6///2X,39HMINIMUM ALLOWED ABSOLUTE VALU 7800000
           3E, AMIN = ,F12.3//2X,35HMAXIMUM ALLOWED DIFFERENCE, AMAX = ,F9.4)  7900000
      C-----                                                                  8000000
      C     SET RADIAL GRID SIZES FOR VARIOUS REGIONS.                        8100000
      C-----                                                                  8200000
000167        IF(NW-NR) 25, 25, 28                                            8300000
000172      25 DELR1 = DELR                                                   8400000
000174         GO TO 30                                                       8500000
```

```
000174      23 DELR1 =  NX*DELR                                          8600000
000177      33 DELR2 = DELR                                              8700000
000201         DELRS1 = DELRS                                            8800000
000202         DELRS2 = NXS*DELRS                                        8900000
000204         DELR22 = DELR2*2.0                                        9000000
000206         DELR24 = DELR2*4.0                                        9100000
000210         DELZZ = DELZ*DELZ                                         9200000
000211         DELZZ6 = 6.0*DELZZ                                        9300000
000213         DELZZ8 = 8.0*DELZZ                                        9400000
        C-----                                                           9500000
        C      STORE CHARACTERISTIC VALUES IN GAS PHASE.                 9600000
        C-----                                                           9700000
        C      INPUT OF CHARACTERISTIC VALUES SHOULD HAVE THE FOLLOWING UNITS=  9800000
        C      RO = FT, VO = FT/SEC, TO = DEGREE R, DENO = LBM/FT/FT/FT, AMU =  9900000
        C      LBM/SEC/FT, DO = FT*FT/SEC, WO = LBM/FT/FT/FT/SEC, ALAMO = BTU/  10000000
        C      HR/FT/DEGREE R, CPO = BTU/LB, PG = PSF/FT.                10100000
        C      PG IS THE FAVORABLE DOWNSTREAM PRESSURE GRADIENT IN THE GAS PHASE.  10200000
        C-----                                                           10300000
000214         READ (5,31) RO, VO, TO, DENO, AMUO, DO, WO, ALAMO, CPO, PG  10400000
000244      31 FORMAT (10F8.0)                                           10500000
        C-----                                                           10600000
        C      STORE COMBUSTION DATA FOR REACTION OF THE FORM=           10700000
        C      OXIDIZER + FUEL = PRODUCT.                                10800000
        C      RA1 AND RA2 ARE RADII OF REACTING MOLECUES.               10900000
        C      E IS THE ACTIVATION ENERGY IN KCAL/G-MOLE.                11000000
        C      SF IS THE STERIC FACTOR.                                  11100000
        C      NU1, NU2 AND NU3 ARE THE STOICHEIOMETRIC COEFFICIENT OF   11200000
        C      OXIDIZER, FUEL AND PRODUCT RESPECTIVELY.                  11300000
        C      TC IS THE MINIMUM TEMPERATURE FOR COMBUSTION TO TAKE PLACE.  11400000
        C      FLL AND FLU ARE LOWER AND UPPER FLAMMABILITY LIMITS RESPECTIVELY  11500000
        C      EXPRESSED AS FRACTION OF THE THEORETICAL FUEL-OXIDIZER RATIO.  11600000
        C-----                                                           11700000
000244         READ(5,31) ANU1,ANU2,ANU3,TC,RA1,RA2,CE,SF,FLL,FLU        11800000
        C-----                                                           11900000
        C      STORE CHARACTERISTIC VALUES IN SOLID PHASE.               12000000
        C-----                                                           12100000
        C      INPUT OF CHARACTERISTIC VALUES SHOULD HAVE THE FOLLOWING UNITS=  12200000
        C      DENSO = LBM/FT/FT/FT, TSO = DEGREE R, ALAMSO = BTU/HR/FT/DEGREE R,  12300000
        C      CSO = BTU/LBM/DEGREE R, RBO = FT/SEC, TSC = DEGREE R.     12400000
        C      TSC IS THE MINIMUM TEMPERATURE FOR THE FUEL TO VAPORIZED. 12500000
        C-----                                                           12600000
000274         READ (5,31) DENSO, TSO, ALAMSO, CSO, RBO,TSC              12700000
        C-----                                                           12800000
```

```
      C     STORE VALUES FOR THE MOLECULAR WEIGHTS , HEAT OF FORMATION AND
      C     OTHER CONSTANTS OF GAS SPECIES.
      C     THESE VALUES SHOULD BE CONSISTENT WITH THE PARTICULAR SPECIES IN
      C     MIND.
      C-----
000314      DO 32 I = 1,NI
000316   32 READ(5,33) AMI(I),CAI(I),CBI(I),CCI(I),HSL(I),HLG(I),HIO(I),TBP(I)
000344   33 FORMAT(3F10.0,F10.0,4F10.0)
000344      TMAX = TBP(3)/TC
      C-----
      C     PRINT CHARACTERISTIC VALUES AND CONSTANTS IN SOLID PHASE.
      C-----
000346      WRITE(6,38) DENSO,TSO,ALAMSO,CSO,RRO,TSC
000365   38 FORMAT(////2X,51HCHARACTERISTIC VALUES AND CONSTANTS IN SOLID PHASE
     1 ,/2X,50H--------------------------------------------------///
     22X,9HDENSO  = ,G11.5,13H LBM/FT/FT/FT,22X,6HTSO = ,G11.4,9H DEGREE
     3 R///2X,9HALAMSO = G11.5,19H BTU/HR/FT/DEGREE R,16X,6HCSO = ,G11.4
     4,17H BTU/LBM/DEGREE R///2X,9HRRO    = ,G11.3,7H FT/SEC,28X,6HTSC =
     5 G12.5,8HDEGREE R)
      C-----
      C     PRINT CHARACTERISTIC VALUES AND CONSTANTS IN GAS PHASE.
      C-----
000365      WRITE (6,41) RO,VC,TO,DENO,AMUO,DO,NO,ALAMO,CPO,PG
000415   41 FORMAT(1H1//2X,49HCHARACTERISTIC VALUES AND CONSTANTS IN GAS PHASE
     1 /2X,48H-------------------------------------------------///
     22X,8HRO     = ,F11.6,3H FT,27X,8HVO     = ,F11.4,7H FT/SEC.//
     32X,8HTO     = ,F11.2,9H DEGREE R,21X,8HDENO  = ,F11.6,13H LBM/FT/FT
     4/FT//2X,8HAMUO  = ,F11.6,11H LBM/SEC/FT,19X,8HDO    = ,F11.6,
     510H FT*FT/SEC//2X,8HWO     = ,F11.6,17H LBM/FT/FT/FT/SEC,13X,
     68HALAMO = ,F11.6,19H BTU/HR/FT/DEGREE R//2X,8HCPO   = ,F11.6,17H B
     7TU/LBM/DEGREE R,13X,8HPG    = ,F11.6,9H PSF./FT.)
000415      DO 42 I = 1, NI
000417   42 WRITE(6,43) I,AMI(I),CAI(I),HSL(I),HLG(I),CBI(I),CCI(I),HIO(I),
     1TBP(I)
000447   43 FORMAT (///2X,8HSPECIES , I2,2H =,2X,6HAMI = ,G12.4,4X,6HCAI = ,
     1G12.5,4X,6HHSL = ,G12.5,8HBTU/LBM ,8X,6HHLG = ,G12.5,8H BTU/LBM/
     22X,12H------------ /16X,6HCBI = ,G12.5,4X,6HCCI = ,G12.5,4X,6HHIO
     3= ,G12.5,8HBTU/LBM ,8X,6HTBP = ,G12.5,8HDEGREE R)
000447      WRITE(6,45) ANU1, ANU2, ANU3, SF, FLL, FLU, TC, RA1, RA2, CE
000476   45 FORMAT(///2X,16HCOMBUSTION DATA /2X,15H--------------- ///
     12X,7HANU1 = ,F6.2,15X,7HANU2 = ,F6.2,15X,7HANU3 = ,F6.2///
     22X,5HSF = ,F8.3,10X,6HFLL  = ,F8.3,10X,6HFLL = ,F8.3,
     310X,5HTC = ,F8.2,9H DEGREE R///
```

```
          40X,6HRA1 = ,F8.4,9H ANGSTROM,10X,6HRA2 = ,F8.4,9H ANGSTROM,10X,
          55HCE = ,F10.3,12H KCAL/G-MOLE )
      C-----
      C      CALCULATE NON-DIMENSIONALIZED GROUPS.
      C-----
000476        RE= DENO*VO*RO/AMUO
000502        SC = AMUO/(DENO*DO)
000504        PR = CPO*AMUO*3600.0/ALAMO
000507        EC = VO*VO/CPO/TO/32.17/778.28
000513        DAM = RO*WO/(DENO*VO)
000516        DENRA = DENSO/DENO
000520        VRA = RRO/VO
000522        TRA = TSO/TO
000524        ALAMRA = ALAMSO/ALAMO
000526        DFURA1 = DO/RO/VO
000530        DFURA2 = DO*DENO*CPO*3600.0/ALAMO
000533        DFURA3 = RO*VO*DENO*CPO*3600.0/ALAMO
000540        DFURA4 = RO*VO*DENSO*CSO*3600.0/ALAMSO
000545        DFURA5 = RO*RRO*DENSO*CSO*3600.0/ALAMSO
000552        DF44 = DFURA4*4.0
000554        RESC8 = RE*SC*8.0
000557        RESC16 = 2.0*RESC8
000560        REPR8 = RE*PR*8.0
      C-----
      C      PRINT VALUES OF NON-DIMENSIONALIZED GROUPS.
      C-----
000562        WRITE(6,50)
000565     50 FORMAT(1H1//2X, 20HCALCULATED CONSTANTS/2X,20H-------------------
          1////40X,30HVALUES OF DIMENSIONLESS GROUPS /40X,30H---------------
          2-------------- ////)
000565        WRITE (6,51) RE, SC, PR, EC, DAM, DFURA1, DFURA2, DFURA3, DFURA4,
          1DFURA5, DENRA, VRA, TRA, ALAMRA
000625     51 FORMAT(19X,10HDENO*VO*RO,46X,10H   AMUO   /10X,9HRE      = ,13H----
          1------ = ,G11.4,23X,9HSC      = ,13H---------- = ,G11.4/19X,10H   A
          2MUO   ,46X,10H DENO*DO  ///19X,10H CPO*AMUO ,46X,10H  VO*VO   /10X
          3,9HPR      = ,13H---------- = ,G11.4,23X,9HEC      = ,13H----------
          4= ,G11.4/19X,10H  ALAMO   ,46X,10H  CPO*TO  ///19X,10H  RO*WO   ,
          546X,10H    DO    /10X,9HDAM     = ,13H---------- = ,G11.4,23X,
          69HDFURA1 = ,13H---------- = ,G11.4/19X,10H DENO*VO  ,46X,10H  RO*V
          7O   ///19X,10H    DO    ,46X,10H  RO*VO   /10X,9HDFURA2 = ,13H----
          8------ = ,G11.4,23X,9HDFURA3 = ,13H---------- = ,G11.4/19X,10H  AL
          9PHAO  ,46X,10H  ALPHAO  ///19X,10H  RO*VO   ,46X,10H  RO*RRO  /10X
          1,9HDFURA4 = ,13H---------- = ,G11.4,23X,9HDFURA5 = ,13H----------
```

```
      2= .G11.4/19X,10H ALPHASO  .46X,10H ALPHASO  ///19X,10H  DENSO    .
      346X,10H    RO     /10X,9HDENRA  = .13H---------- = .G11.4.23X.
      4SHVRA     = .13H---------- = .G11.4/19X,10H   DENO    .46X,10H     VO
      5    ///19X,10H   TSO     .46X,10H  ALAMSO  /10X,9HTRA     = .13H----
      6------ = .G11.4.23X,9HALAMRA = .13H---------- = .G11.4/19X,10H
      7TO    .46X,10H  ALAMO    )
C-----
C     SET VALUE FOR UNIVERSAL GAS CONSTANT.
C-----
      CCR = 1.987
C-----
C     STORE INITIAL CONDITIONS (L=1).
C     ALL DEPENDENT VARIABLES ARE NON-DIMENSIONALIZED.
C     IT IS REQUIRED THAT THE RADIAL VELOCITY IS ZERO AT M=1
C     AND THE AXIAL VELOCITY IS ZERO AT M= NW.
C     THEN STORE ALL GUESS VALUES FOR THE DEPENDENT VARIABLES AT L = 2.
C     IT IS REQUIRED THAT THE RADIAL VELOCITY IS ZERO AT M = 1 AND
C     THE AXIAL VELOCITY IS ZERO AT M = NW. THE BOUNDARY TEMPERATURE
C     IN THE SOLID PHASE IS ASSUMED TO BE CONSTANT.
C-----
C     IF TIME = ZERO, READ ADDITIONAL DATA FROM CARDS.
C     OTHERWISE, READ FROM TAPE.
C-----
      IF(TIME-0.0) 85, 60, 85
C-----
C     READ DATA FROM CARDS.
C-----
   60 TIME1 = 0.0
      READ(5,61) (( VR(1,M,N), N = 1, NZ), M = 1, NW)
      READ(5,61) ((T(1,M,N), N = 1, NZ), M = 1, NW)
      READ (5,61) ((TS(1,MS,N) , N=1, NZ), MS=1,NWS)
      READ (5,61)  (((YI(I,M,N), N=1,NZ), M=1,NW), I=1,NI)
   61 FORMAT (10F8.0)
C-----
C     CALCULATE PRESSURE BASED ON A FAVORABLE DOWNSTREAM PRESSURE
C     GRADIENT.
C-----
      PINLET = CCR/(CFO*FO*AMI(1))
      DELP = 32.17*DELZ*RO*PG/(DENO*VO*VO)
      DO 70 M = 1, NW
      P(1,M,1) = PINLET
      DO 70 N = 2, NZ
      NB = N - 1
```

```
000760          P(1,M,N) = P(1,M,NB) - DELP
000770       70 CONTINUE
          C-----
          C     STORE AXIAL VELOCITY VALUES.
          C-----
000774          CALL VEL(VZ,NW,NZ,NR,DELR1,DELR2)
          C-----
          C     INITIAL DENSITY OF GAS MIXTURE IS CALCULATED FROM EQUATION OF
          C     STATE FOR IDEAL GAS MIXTURE.
          C-----
001000          DO 74 N = 1, NZ
001002          DO 74 M = 1, NW
001003          SUMD = 0.0
001004          DO 72 I = 1, NI
001006       72 SUMD = YI1(I,M,N)/AMI(I)+SUMD
001020       74 DEN(1,M,N) = P(1,M,N)*CPO*EC/(CCR*T(1,M,N)*SUMD)
001042          DO 75 M = 1, NW
001043          DEN(2,M,1) = DEN(1,M,1)
001050       75 CONTINUE
          C-----
          C     CALCULATE ALL NON-DIMENSIONALIZED FUNCTIONS FOR L=1.
          C-----
001052          CALL SUB1(1,YI1)
          C-----
          C     CALCULATE RADIAL VELOCITY AT INTERFACE.
          C     SET GUESS VALUES FOR DEPENDENT VARIABLES.
          C-----
001054          DO 82 N = 1, NZ
001056          Y = (DI1(2,NW,N)+DI1(2,NW1,N))*(YI1(2,NW,N)-YI1(2,NW1,N))/DELR22
001075          VR(1,NW,N) = DELRA1*Y-VRA*DENRA*DENS(1,1,N)*RR(1,N)/DEN(1,NW,N)
001114          VR(2,NW,N) = VR(1,NW,N)
001120          DO 78 M = 1, NW1
001122          VR(1,M,N) = VR(1,M,N)*VR(1,NW,N)
001131          VR(2,M,N) = VR(1,M,N)
001136       78 CONTINUE
001140          DO 80 MS = 1, NWS
001142       80 TS(2,MS,N) = TS(1,MS,N)
001155          DO 82 M =1, NW
001156          T(2,M,N) = T(1,M,N)
001165          P(2,M,N) = P(1,M,N)
001170          DO 82 I = 1, NI
001172          YI2(I,M,N) = YI1(I,M,N)
001204       82 CONTINUE
```

```
      C-----
      C     PUNCH OUT INITIAL VALUES OF ALL DEPENDENT VARIABLES FOR PLOTTING.
      C-----
001213        DO 84 N = 1, NZ, 3
001215        PUNCH 2100, (DEN(I,M,N), M = 1, NW), TIME, N
001234        PUNCH 2100, ( VR(I,M,N), M = 1, NW), TIME, N
001254        PUNCH 2100, ( VZ(I,M,N), M = 1, NW), TIME, N
001274        PUNCH 2100, (  T(I,M,N), M = 1, NW), TIME, N
001314        DO 83 I = 1, NI
001316     83 PUNCH 2100, (YI1(I,M,N), M = 1, NW), TIME, N
001341        PUNCH 2400, ( TS(I,M,N), M = 1, NWS), TIME, N
001360     84 CONTINUE
001363        GO TO 95
      C-----
      C     READ DATA FROM TAPE.
      C-----
001363     85 REWIND 22
001365        DO 90 I = 1, NI
001367        READ(22)((YI1(I,M,N), N = 1, NZ), M = 1, NW)
001407        READ(22)((YI2(I,M,N), N = 1, NZ), M = 1, NW)
001427     90 CONTINUE
001432        DO 92 L = 1, 2
001433        READ(22)((DEN(L,M,N), N =1, NZ), M = 1,NW)
001453        READ(22)(( VR(L,M,N), N =1, NZ), M = 1,NW)
001473        READ(22)(( VZ(L,M,N), N =1, NZ), M = 1,NW)
001513        READ(22)((  T(L,M,N), N =1, NZ), M = 1,NW)
001533        READ(22)((  P(L,M,N), N =1, NZ), M = 1,NW)
001553        READ(22)((   TS(L,MS,N), N = 1, NZ), MS = 1, NWS)
001572        READ(22)(( DENS(L,MS,N), N = 1, NZ), MS = 1, NWS)
001611        READ(22)((ALAMS(L,MS,N), N = 1, NZ), MS = 1, NWS)
001630        READ(22)((   CS(L,MS,N), N = 1, NZ), MS = 1, NWS)
001647     92 CONTINUE
001651        READ(22) TIME1,((RR(L,N), N = 1, NZ), L = 1, 2), (R(M), M =1, NW)
      C-----
      C     CALCULATE ALL NON-DIMENSIONALIZED FUNCTIONS FOR I = 1.
      C-----
001677        CALL SUB1(1,YI1)
      C-----
      C     PRINT OUT INITIAL VALUES OF ALL DEPENDENT VARIABLES.
      C-----
001701     95 TIME =TIME1
001703        CALL FORM1(1,YI1)
      C-----
```

```
      C     PRINT OUT ALL NON-DIMENSIONALIZED FUNCTIONS FOR I=1.
      C-----
001705      L = 1
001706      CALL FORM2(1,YI1,CI1,WI1,CPI1,HI1)
      C-----
      C     PRINT OUT GUESS VALUES OF ALL DEPENDENT VARIABLES AT TIME STEP 2.
      C-----
      C     CALL FORM1(2,YI2)
      C-----
      C     CALCULATE VALUES OF ALL DEPENDENT VARIABLES FOR EACH UNKNOWN
      C     TIME STEP.
      C-----
001712      ADELT = DELT*RO/VC
001715      DO 990 L = 2, NT1
      C-----
      C     INITIATE ITERATION.
      C-----
001716      IT = 0
001717  125 IT = IT + 1
      C-----
      C     CALCULATE DENSITY FROM EQUATION OF STATE FOR IDEAL GAS MIXTURE.
      C-----
001721      DO 250 N = 2, NZ
001722      DO 250 M =1,NW
001723      SUMD = 0.0
001724      DO 250 I = 1, NI
001726  250 SUMD = YI2(I,M,N)/AMI(I)+SUMD
001740  250 DEN(2,M,N) = P(2,M,N)*CPO*FC/(CCR*T(2,M,N)*SUMD)
      C-----
      C     CALCULATE ALL NON-DIMENSIONALIZED FUNCTIONS AT UNKNOWN TIME STEP.
      C-----
001762      CALL SUB1(2,YI2)
      C-----
      C     CALCULATE RADIAL VELOCITY AT INTERFACE.
      C-----
001764      DO 230 N = 2, NZ
001766      Y = (DI2(2,NW,N)+DI2(2,NW1,N))*(YI2(2,NW,N)-YI2(2,NW1,N))/DELR22
002005      TEMPR(NW,N) = DEURA1*Y-DENRA*VRA*DENS(2,1,N)*RR(2,N)/DEN(2,NW,N)
002023  230 CONTINUE
      C
002026      DELR = DELR1
      C
      C-----
```

```
      C     CALCULATE AXIAL VELOCITY FROM Z-MOMENTUM EQUATION.                38700000
      C     CALCULATE RADIAL VELOCITY FROM R-MOMENTUM EQUATION.               38800000
      C     CALCULATE TEMPERATURE FROM ENERGY EQUATIONS.                      38900000
      C-----                                                                  39000000
002027        DO 320 M = 2, NM1                                               39100000
002031        IF(M - NR) 284, 282, 284                                        39200000
002033    282 DELR = DEL22                                                    39300000
002035    284 RB = DELR/R(M)                                                  39400000
002040        MA = M+1                                                        39500000
002041        MB = M-1                                                        39600000
002042        MC = M-2                                                        39700000
002043        RC = DELR/(R(M)+R(MB))                                          39800000
002047        RC22 = RC/2.0                                                   39900000
002051        RC33 = RC/3.0                                                   40000000
002052        RC4 = 4.0*RC                                                    40100000
002054        DELRR = DELR*DELR                                               40200000
002055        DELR7 = DELR*DEL7                                               40300000
002057        DELRR6 = 6.0*DELRR                                              40400000
002061        DELRR8 = 8.0*DELRR                                              40500000
002062        DO 320 N = 2, NZ                                                40600000
002064        NA = N+1                                                        40700000
002066        NB = N-1                                                        40800000
002067        NC = N-2                                                        40900000
002070        X = UCT(M,N,DEN)                                                41000000
002074        Y = UCT(M,N,VR)                                                 41100000
002077        Z = UCT(M,N,VZ)                                                 41200000
002102        S = UCT(M,N,AMU)                                                41300000
002105        XC = X*UCT(M,N,CP)                                              41400000
002111        ALAMU = UCT(M,N,ALAM)                                           41500000
002114        FUR = URCT(M,N,P)                                               41600000
002117        FUZ = UZCT(M,N,P)                                               41700000
002122        FYZ = 0.25*(Y/DELR+Z/DEL7)                                      41800000
002126        AMU233 = AMU(2,M,N)                                             41900000
002133        AMU133 = AMU(1,M,N)                                             42000000
002136        AMU232 = AMU(2,M,NB)                                            42100000
002142        AMU132 = AMU(1,M,NB)                                            42200000
002146        AMU223 = AMU(2,MB,N)                                            42300000
002152        AMU123 = AMU(1,MB,N)                                            42400000
002156        AMU222 = AMU(2,MB,NB)                                           42500000
002161        AMU122 = AMU(1,MB,NB)                                           42600000
002165        VR243 = VR(2,MA,N)                                              42700000
002171        VR143 = VR(1,MA,N)                                              42800000
002174        VR242 = VR(2,MA,NB)                                             42900000
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002200        VR142 = VR(1,MA,NB)                                          43000000
002203        VR233 = VR(2,M,N)                                            43100000
002207        VR133 = VR(1,M,N)                                            43200000
002213        VR232 = VR(2,M,NB)                                           43300000
002216        VR132 = VR(1,M,NB)                                           43400000
002222        VR223 = VR(2,MB,N)                                           43500000
002226        VR123 = VR(1,MB,N)                                           43600000
002231        VR222 = VR(2,MB,NB)                                          43700000
002235        VR122 = VR(1,MB,NB)                                          43800000
002240        VZ243 = VZ(2,MA,N)                                           43900000
002244        VZ143 = VZ(1,MA,N)                                           44000000
002250        VZ242 = VZ(2,MA,NB)                                          44100000
002253        VZ142 = VZ(1,MA,NB)                                          44200000
002257        VZ233 = VZ(2,M,N)                                            44300000
002263        VZ133 = VZ(1,M,N)                                            44400000
002266        VZ232 = VZ(2,M,NB)                                           44500000
002272        VZ132 = VZ(1,M,NB)                                           44600000
002275        VZ223 = VZ(2,MB,N)                                           44700000
002301        VZ123 = VZ(1,MB,N)                                           44800000
002305        VZ222 = VZ(2,MB,NB)                                          44900000
002310        VZ122 = VZ(1,MB,NB)                                          45000000
002314        T221 = T(2,M,NB)                                             45100000
002320        T212 = T(2,MB,N)                                             45200000
002323        T211 = T(2,MB,NB)                                            45300000
002327        T122 = T(1,M,N)                                              45400000
002333        T121 = T(1,M,NB)                                             45500000
002337        T112 = T(1,MB,N)                                             45600000
002343        T111 = T(1,MB,NB)                                            45700000
002346        ALAM222 = ALAM(2,M,N)                                        45800000
002352        ALAM221 = ALAM(2,M,NB)                                       45900000
002356        ALAM212 = ALAM(2,MB,N)                                       46000000
002362        ALAM211 = ALAM(2,MB,NB)                                      46100000
002365        ALAM122 = ALAM(1,M,N)                                        46200000
002371        ALAM121 = ALAM(1,M,NB)                                       46300000
002375        ALAM112 = ALAM(1,MB,N)                                       46400000
002401        ALAM111 = ALAM(1,MB,NB)                                      46500000
002404        SUM1 = 0.0                                                   46600000
002405        SUM2 = 0.0                                                   46700000
002406        SUM3 = 0.0                                                   46800000
002407        DO 290 I = 1 , NI                                            46900000
002410        DC = UCTI(I,M,N,DI1,DI2)*UCTI(I,M,N,CPI1,CPI2)               47000000
002421        SUM1 = SUM1 + UCTI(I,M,N,HI1,HI2)*UCTI(I,M,N,WI1,WI2)        47100000
002433        SUM2 = SUM2+DC*(YI2(I,M,N)+YI2(I,M,NB)-YI2(I,MB,N)-YI2(I,MB,NB)  47200000
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                1+YI1(I,M,N)+YI1(I,M,NB)-YI1(I,MB,N)-YI1(I,MB,NB))                47300000
002472            SUM3 = SUM3+DC*(YI2(I,M,N)-YI2(I,M,NB)+YI2(I,MB,N)-YI2(I,MB,NB)  47400000
                1+YI1(I,M,N)-YI1(I,M,NB)+YI1(I,MB,N)-YI1(I,MB,NB))                47500000
002523      230 CONTINUE                                                          47600000
002526          IF(M-2) 296, 294, 296                                             47700000
002530      294 VR213 = VR(2,M,N)                                                 47800000
002535          VR113 = VR(1,M,N)                                                 47900000
002540          VR212 = VR(2,M,NB)                                                48000000
002544          VR112 = VR(1,M,NB)                                                48100000
002550          VZ213 = VZ(2,M,N)                                                 48200000
002554          VZ113 = VZ(1,M,N)                                                 48300000
002557          VZ212 = VZ(2,M,NB)                                                48400000
002563          VZ112 = VZ(1,M,NB)                                                48500000
002567          T202 = T(2,M,N)                                                   48600000
002573          T201 = T(2,M,NB)                                                  48700000
002577          T102 = T(1,M,N)                                                   48800000
002603          T101 = T(1,M,NB)                                                  48900000
002607          R2 = 0.0                                                          49000000
002610          GO TO 298                                                         49100000
002610      296 R2 = DELR/R(MB)                                                   49200000
002613          VR213 = VR(2,MC,N)                                                49300000
002617          VR113 = VR(1,MC,N)                                                49400000
002623          VR212 = VR(2,MC,NB)                                               49500000
002627          VR112 = VR(1,MC,NB)                                               49600000
002632          VZ213 = VZ(2,MC,N)                                                49700000
002636          VZ113 = VZ(1,MC,N)                                                49800000
002642          VZ212 = VZ(2,MC,NB)                                               49900000
002646          VZ112 = VZ(1,MC,NB)                                               50000000
002651          T202 = T(2,MC,N)                                                  50100000
002655          T201 = T(2,MC,NB)                                                 50200000
002661          T102 = T(1,MC,N)                                                  50300000
002665          T101 = T(1,MC,NB)                                                 50400000
002671      298 IF(N-2) 304, 302, 304                                             50500000
002673      302 VR231 = 2.0*VR(2,M,1)-VR(2,M,2)                                   50600000
002700          VR131 = 2.0*VR(1,M,1)-VR(1,M,2)                                   50700000
002703          VR121 = 2.0*VR(1,MB,1)-VR(1,MB,2)                                 50800000
002710          VR221 = 2.0*VR(2,MB,1)-VR(2,MB,2)                                 50900000
002713          VZ231 = 2.0*VZ(2,M,1)-VZ(2,M,2)                                   51000000
002716          VZ131 = 2.0*VZ(1,M,1)-VZ(1,M,2)                                   51100000
002721          VZ121 = 2.0*VZ(1,MB,1)-VZ(1,MB,2)                                 51200000
002725          VZ221 = 2.0*VZ(2,MB,1)-VZ(2,MB,2)                                 51300000
002730          T220 = 2.0*T(2,M,1)-T(2,M,2)                                      51400000
002734          T210 = 2.0*T(2,MB,1)-T(2,MB,2)                                    51500000
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002740          T120 = 2.0*T(1,M,1)-T(1,M,2)                                    51600000
002743          T110 = 2.0*T(1,MB,1)-T(1,MB,2)                                  51700000
002747          GO TO 306                                                       51800000
002750      304 VR231 = VR(2,M,NC)                                              51900000
002755          VR131 = VR(1,M,NC)                                              52000000
002760          VR221 = VR(2,MB,NC)                                             52100000
002764          VR121 = VR(1,MB,NC)                                             52200000
002770          VZ231 = VZ(2,M,NC)                                              52300000
002774          VZ131 = VZ(1,M,NC)                                              52400000
002777          VZ221 = VZ(2,MB,NC)                                             52500000
003003          VZ121 = VZ(1,MB,NC)                                             52600000
003007          T220 = T(2,M,NC)                                                52700000
003013          T210 = T(2,MB,NC)                                               52800000
003016          T120 = T(1,M,NC)                                                52900000
003022          T110 = T(1,MB,NC)                                               53000000
003026      306 IF(N-NZ) 310, 308, 310                                          53100000
003030      308 VR234 = 2.0*VR(2,M,NZ)-VR(2,M,NZ1)                              53200000
003041          VR134 = 2.0*VR(1,M,NZ)-VR(1,M,NZ1)                              53300000
003051          VR224 = 2.0*VR(2,MB,NZ)-VR(2,MB,NZ1)                            53400000
003062          VR124 = 2.0*VR(1,MB,NZ)-VR(1,MB,NZ1)                            53500000
003072          VZ124 = 2.0*VZ(1,MB,NZ)-VZ(1,MB,NZ1)                            53600000
003101          VZ224 = 2.0*VZ(2,MB,NZ)-VZ(2,MB,NZ1)                            53700000
003110          VZ134 = 2.0*VZ(1,M,NZ)-VZ(1,M,NZ1)                              53800000
003120          VZ234 = 2.0*VZ(2,M,NZ)-VZ(2,M,NZ1)                              53900000
003127          T223 = 2.0*T(2,M,NZ)-T(2,M,NZ1)                                 54000000
003136          T213 = 2.0*T(2,MB,NZ)-T(2,MB,NZ1)                               54100000
003146          T123 = 2.0*T(1,M,NZ)-T(1,M,NZ1)                                 54200000
003156          T113 = 2.0*T(1,MB,NZ)-T(1,MB,NZ1)                               54300000
003166          GO TO 312                                                       54400000
003166      310 VR234 = VR(2,M,NA)                                              54500000
003173          VR134 = VR(1,M,NA)                                              54600000
003176          VR224 = VR(2,MB,NA)                                             54700000
003202          VR124 = VR(1,MB,NA)                                             54800000
003206          VZ234 = VZ(2,M,NA)                                              54900000
003212          VZ134 = VZ(1,M,NA)                                              55000000
003215          VZ224 = VZ(2,MB,NA)                                             55100000
003221          VZ124 = VZ(1,MB,NA)                                             55200000
003225          T223 = T(2,M,NA)                                                55300000
003231          T213 = T(2,MB,NA)                                               55400000
003234          T123 = T(1,M,NA)                                                55500000
003240          T113 = T(1,MB,NA)                                               55600000
003244      312 ZR2ORD = (S*((VR232-VR233)+(VR222-VR223)+(VR132-VR133)+(VR122   55700000
               1-VR123))*RC22+(AMU233*(VR243-VR223)+AMU232*(VR222-VR242)+       55800000
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     2AMU223*(VR233-VR213)+AMU222*(VR212-VR232)+AMU133*(VR143-VR123)+
     3AMU132*(VR122-VR142)+AMU123*(VR133-VR113)+AMU122*(VR112-VR132))
     4/12.0+(AMU233*(VR232-VR234)+AMU232*(VR231-VR233)+AMU223*(VR224-
     5VR222)+AMU222*(VR223-VR221)+AMU133*(VR132-VR134)+AMU132*(VR131-
     6VR133)+AMU123*(VR124-VR122)+AMU122*(VR123-VR121))/8.0+(((AMU233*
     7VR233-AMU232*VR232)+(AMU133*VR133-AMU132*VR132))*R3+((AMU223*VR223
     8-AMU222*VR222)+(AMU123*VR123-AMU122*VR122))*R2)/6.0)/DELR7
003412  ZZ2ORD = (((S*RC4*((VZ232-V7222)+(V7133-V7123)+(V7132-V7122))+
     1AMU233*(V7243-V7223)+AMU232*(V7242-V7222)+AMU222*
     2(V7212-V7232)+AMU133*(VZ143-VZ123)+AMU132*(V7142-V7122)+AMU123*
     3(V7113-VZ133)+AMU122*(VZ112-V7132))/DELRR8+(AMU233*(V7234-
     4V7232)+AMU223*(V7224-VZ222)+AMU222*(V7221-V7223)+
     5AMU133*(VZ134-V7132)+AMU132*(V7131-V7133)+AMU123*(V7124-V7122)+
     6AMU122*(V7121-V7123))/DELZ76)+AMU232*V7231/DELZ76+(AMU223*V7213-
     7S*RC4*V7223)/DELRR8
003525  ZDE = (((AMU223-S*RC4)/DELRR8+AMU232/DELZ76)/RE+X*FY7)+FT*X
003537  TEMPZ(M,N) = (((-PUZ+(ZZ2ORD-ZR2ORD)/RE)-0.25*X*(Y*((V7232-V7222)+
     1(V7133-VZ123)+(V7132-V7122)-VZ223)/DELR+7*((V7223-V7222)+(V7133-
     2V7132)+(VZ123-VZ122)-V7232)/DELZ))-FT*((V7232-V7132)+(V7223-V7123)
     3+(VZ222-V7122)-V7133)*X)/ZDE
C
003612  RZ2ORD=(S*(V7232-V7233-V7223+V7222-VZ133+V7132-V7123+V7122)*RC33
     1+(AMU233*(V7243-V7223)+AMU232*(V7222-V7242)+AMU223*(V7233-V7213)+
     2AMU222*(V7212-V7232)+AMU133*(V7143-VZ123)+AMU132*(V7122-V7142)+
     3AMU123*(V7133-V7113)+AMU122*(V7112-V7132))/8.0+(AMU233*(V7232-
     4V7234)+AMU232*(VZ231-V7233)+AMU223*(V7224-VZ222)+AMU222*(V7223-
     5V7221)+AMU133*(V7132-V7134)+AMU132*(V7131-V7133)+AMU123*(V7124-
     6V7122)+AMU122*(V7123-V7121))/12.0)/DELR7
003727  RR2ORD = (S*2.0*(2.0*((VR232-VR222)+(VR133-VR123)+(VR132-VR122)
     1-VR223)-(VR232+VR223+VR222+VR133+VR132+VR123+VR122)*RC)*RC
     2-(AMU232*VR232+AMU133*VR133+AMU132*VR132)*R3+(AMU223*VR223+
     3AMU222*VR222+AMU123*VR123+AMU122*VR122)*R2+AMU223*VR213+(AMU233*
     4(VR243-VR223)+AMU232*(VR242-VR222)+AMU222*(VR212-VR232)+AMU133*
     5(VR143-VR123)+AMU132*(VR142-VR122)+AMU123*(VR113-VR133)+AMU122*
     6(VR112-VR132)))/DELRR6+(AMU232*VR231+(AMU233*(VR234-VR232)+AMU223*
     7(VR224-VR222)+AMU222*(VR221-VR223)+AMU133*(VR134-VR132)+AMU132*
     8(VR131-VR133)+AMU123*(VR124-VR122)+AMU122*(VR121-VR123)))/DELZ78
004067  RDE =(((AMU223+AMU233*R3-S*(8.-RC4)*RC22)/DELRR6+AMU232/DELZ78)/RE
     1+X*FYZ)+FT*X
004105  TEMPR(M,N) = (((-PUR+(RZ2ORD+RR2ORD)/RE)-0.25*X*(Y*((VR232-VR222)+
     1(VR133-VR123)+(VR132-VR122)-VR223)/DELR+7*((VR223-VR222)+(VR133-
     2VR132)+(VR123-VR122)-VR232)/DELZ))-FT*((VR232-VR132)+(VR223-VR123)
     3+(VR222-VR122)-VR133)*X)/RDE
```

```
004157          T2ORD = ((ALAM222*(T(2,MA,N)-T212)+ALAM221*(T(2,MA,NB)-T211)+
               1ALAM211*(T201-T221)+ALAM122*(T(1,MA,N)-T112)+ALAM121*(T(1,MA,NB)-
               2T111)+ALAM112*(T102-T122)+ALAM111*(T101-T121))/DELRR+(ALAM222*
               3(T223-T221)+ALAM221*T220+ALAM212*(T213-T211)+ALAM211*(T210-T212)+
               4ALAM122*(T123-T121)+ALAM121*(T120-T122)+ALAM112*(T113-T111)+
               5ALAM111*(T110-T112))/DELZZ)+ALAM212*T202/DELRR+ALAM221*T220/DELZZ
004272          PT = P(2,M,N)-P(1,M,N)+P(2,M,NB)-P(1,M,NB)+P(2,MB,N)-P(1,MB,N)+
               1P(2,MB,NB)-P(1,MB,NB)
004316          TDF=((((ALAM212-ALAMU*RC4)/DELRR+ALAM221/DELZZ)/REPRR-
               1X*(SUM2/DELRR+SUM3/DELZZ)/RESC16)+XC*FYZ)+XC*FT
004340          TEMPT(M,N) = ((((T2ORD+ALAMU*((T221-T211)+(T122-T112)+(T121-T111)-
               1T212)*RC4)/REPRR+X*((SUM2/DELRR-SUM3/DELZZ)*((T221-T212)+(T121-T11
               22))+(SUM2/DELRR+SUM3/DELZZ)*((T122-T111)-T211))/RESC16-DAM*SUM1+FC
               3*(Y*PUR+Z*PUZ+PT*FT))-0.25*XC*(Y*(((T221-T211)+(T122-T112)+(T121-
               4T111)-T212)/DELR+Z*(((T212-T211)+(T122-T121)+(T112-T111)-T121)/DELZ
               5))-FT*XC*(((T221-T121)+(T212-T112)+(T211-T111)-T122))/TDF
004450          IF(TEMPR(M,N)-TEMPR(NW,N)) 314, 316, 316
004456      314 TEMPR(M,N) = TEMPR(NW,N)
004464      316 IF(TEMPT(M,N) -TMAX) 320, 320, 318
004471      318 TEMPT(M,N) = TMAX
004475      320 CONTINUE
        C-----
        C       CALCULATE TEMPERATURE IN SOLID PHASE.
        C       AN IMPLICIT CRANK-NICOLSON SCHEME WAS USED.
        C-----
004502          DO 505 MS = 2, NWS1
004504          IF(MS -NRS) 503, 502, 502
004506      502 DELRS = DELRS2
004510          RS = 1.0+(NRS-2)*DELRS1+(MS-NRS+1)*DELRS2
004522          GO TO 504
004522      503 RS = 1.0+(MS-1)*DELRS1
004530      504 MA = MS+1
004532          MB = MS-1
004533          DELRRS = DELRS*DELRS
004534          DO 505 N = 2, NZ1
004536          NA = N+1
004540          NB = N-1
004541          X = (DENS(2,MS,N)+DENS(1,MS,N))/2.0
004551          Y = (CS(2,MS,N)+CS(1,MS,N))/2.0
004556          Z = (ALAMS(2,MS,N)+ALAMS(1,MS,N))/2.0
004564          TEMPS(MS,N) = (X*Y*TS(1,MS,N)/DELT+(((ALAMS(2,MA,N)+ALAMS(1,MA,N))
               1*(TS(2,MA,N)+TS(1,MA,N)-TS(1,MS,N))+(ALAMS(2,MB,N)+ALAMS(1,MB,N))*
               2(TS(2,MB,N)+TS(1,MB,N)-TS(1,MS,N))+Z*(TS(2,MA,N)+TS(1,MA,N)-
```

```
          3TS(2,MB,N)-TS(1,MB,N))/RS)/DELRRS+((ALAMS(2,MS,NA)+ALAMS(1,MS,NA))
          4*(TS(2,MS,NA)+TS(1,MS,NA)-TS(1,MS,N))+(ALAMS(2,MS,NB)+ALAMS(1,MS,
          5NB))*(TS(2,MS,NB)+TS(1,MS,NB)-TS(1,MS,N)))/DEL77)/DF44)
          6/(X*Y/DELT+((ALAMS(2,MA,N)+ALAMS(1,MA,N)+ALAMS(2,MB,N)+ALAMS(1,MB,
          7N))/DELRRS+(ALAMS(2,MS,NA)+ALAMS(1,MS,NA)+ALAMS(2,MS,NB)+
          8ALAMS(1,MS,NB))/DEL77)/DF44)
004725      505 CONTINUE
      C-----
      C       CALCULATE TEMPERATURE FROM BOUNDARY EQUATIONS.
      C       A TIME-INDEPENDENT FINITE DIFFERENCE SCHEME WAS USED.
      C-----
004732          DO 520 N = 2, N7
004734          TEMPT(1,N) = TEMPT(2,N)
004741          SUM1 = 0.0
004741          SUM2 = 0.0
004742          SUM3 = 0.0
004743          DO 515 I = 1,NI
004744          S = HI2(I,NW,N) + HI2(I,NW1,N)
004755          SUM1 = SUM1+S*(DI2(I,NW,N)+DI2(I,NW1,N))*(YI2(I,NW,N)-YI2(I,NW1,N)
         1)/DELR24
004774          SUM2 = SUM2+0.25*S*(YI2(I,NW,N)+YI2(I,NW1,N))
005004          SUM3 = SUM3 + YI2(I,NW,N)*HSGI(2,I,N)
005014      515 CONTINUE
005016          X = 0.5*(DEN(2,NW,N)+DEN(2,NW1,N))
005027          Y = 0.5*(ALAM(2,NW,N)+ALAM(2,NW1,N))
005035          Z = 0.5*(VR(2,NW,N)+VR(2,NW1,N))
005043          XS = DENS(2,1,N)
005046          YS = (ALAMS(2,1,N)+ALAMS(2,2,N))/2.0
005053          TEMPT(NW,N)=(TRA*ALAMRA*(YS*TS(2,2,N)/DELRS1+XS*PR(2,N)*DEURA5*
         1SUM3)+X*(Z*DEURA3*SUM2-DEURA2*SUM1)+Y*T(2,NW1,N)/DELR2)/
         2(Y/DELR2+ALAMRA*YS/DELRS1)
      C
      C-----
      C       SET UPPER AND LOWER BOUNDS FOR TEMPERATURES AT THE BOUNDARY.
      C-----
005110          IF(TEMPT(NW,N)-TEMPT(NW1,N)) 518, 518, 517
005116      517 TEMPT(NW,N) = TEMPT(NW1,N)
005124      518 IF(TEMPT(NW,N)-TSC/TO) 519, 520, 520
005132      519 TEMPT(NW,N) = TSC/TO
005137      520 TEMPS(1,N) = TEMPT(NW,N)/TRA
005147          DO 521 MS = 1, NWS1
005151          TEMPS(MS,N7) = TEMPS(MS,N71)
005157      521 CONTINUE
```

```
      C
005161        DELR = DELR1
      C
      C-----
      C       CALCULATE MASS FRACTION OF SPECIES FROM SPECIES CONTINUITY
      C       EQUATIONS.
      C-----
005163        DO 560 M = 2, NW1
005164        MA = M + 1
005166        MB = M - 1
005167        MC = M - 2
005170        IF(M - NP) 532, 530, 532
005172    530 DELR = DELR2
005174    532 DELRR = DELR*DELR
005176        RC = DELR/(R(M)+R(MB))
005201        RC4 = 4.0*RC
005203        DO 560 N = 2, NZ
005204        NA = N + 1
005206        NB = N - 1
005207        NC = N - 2
005210        S = UCT(M,N,DEN)
005214        Y = UCT(M,N,VR)
005217        Z = UCT(M,N,VZ)
005222        F1 = 0.25*S*(Y/DELR+Z/DELZ)
005227        F2 = S*FT
005230        DO 560 I = 1, NI
005232        IF(M-2) 536, 534, 536
005234    534 YI213 = YI2(I,M,N)
005242        YI212 = YI2(I,M,NB)
005246        YI113 = YI1(I,M,N)
005253        YI112 = YI1(I,M,NB)
005257        GO TO 538
005260    536 YI213 = YI2(I,MC,N)
005266        YI212 = YI2(I,MC,NB)
005272        YI113 = YI1(I,MC,N)
005277        YI112 = YI1(I,MC,NB)
005303    533 IF(N-2) 544, 542, 544
005305    542 YI231 = 2.0*YI2(I,M,1)-YI2(I,M,2)
005313        YI221 = 2.0*YI2(I,MB,1)-YI2(I,MB,2)
005321        YI131 = 2.0*YI1(I,M,1)-YI1(I,M,2)
005325        YI121 = 2.0*YI1(I,MB,1)-YI1(I,MB,2)
005331        GO TO 546
005331    544 YI231 = YI2(I,M,NC)
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005337          YI221 = YI2(I,MB,NC)                                            73100000
005343          YI131 = YI1(I,M,NC)                                             73200000
005347          YI121 = YI1(I,MB,NC)                                            73300000
005353      546 IF(N-NZ) 550, 548, 550                                          73400000
005355      548 YI234 = 2.0*YI2(I,M,NZ)-YI2(I,M,NZ1)                            73500000
005367          YI224 = 2.0*YI2(I,MB,NZ)-YI2(I,MB,NZ1)                          73600000
005401          YI134 = 2.0*YI1(I,M,NZ)-YI1(I,M,NZ1)                            73700000
005412          YI124 = 2.0*YI1(I,MB,NZ)-YI1(I,MB,NZ1)                          73800000
005423          GO TO 552                                                       73900000
005424      550 YI234 = YI2(I,M,NA)                                             74000000
005432          YI224 = YI2(I,MB,NA)                                            74100000
005436          YI134 = YI1(I,M,NA)                                             74200000
005442          YI124 = YI1(I,MB,NA)                                            74300000
005446      552 C = RC4*S*UCTI(I,M,N,DI1,DI2)                                   74400000
005455          DD233 = DEN(2,M,N)*DI2(I,M,N)                                   74500000
005465          DD133 = DEN(1,M,N)*DI1(I,M,N)                                   74600000
005474          DD232 = DEN(2,M,NB)*DI2(I,M,NB)                                 74700000
005503          DD132 = DEN(1,M,NB)*DI1(I,M,NB)                                 74800000
005512          DD223 = DEN(2,MB,N)*DI2(I,MB,N)                                 74900000
005522          DD123 = DEN(1,MB,N)*DI1(I,MB,N)                                 75000000
005531          DD222 = DEN(2,MB,NB)*DI2(I,MB,NB)                               75100000
005541          DD122 = DEN(1,MB,NB)*DI1(I,MB,NB)                               75200000
005550          YI232 = YI2(I,M,NB)                                             75300000
005555          YI223 = YI2(I,MB,N)                                             75400000
005562          YI222 = YI2(I,MB,NB)                                            75500000
005566          YI133 = YI1(I,M,N)                                              75600000
005573          YI132 = YI1(I,M,NB)                                             75700000
005600          YI123 = YI1(I,MB,N)                                             75800000
005605          YI122 = YI1(I,MB,NB)                                            75900000
005611          Y2RD = ((DD233*(YI2(I,MA,N)-YI223)+DD232*(YI2(I,MA,NB)-YI222)+  76000000
               1DD222*(YI212-YI232)+DD133*(YI1(I,MA,N)-YI123)+DD132*(YI1(I,MA,NB)-  76100000
               2YI122)+DD123*(YI113-YI133)+DD122*(YI112-YI132))/DELRR+          76200000
               3(DD233*(YI234-YI232)+DD223*(YI224-YI222)+DD222*(YI221-YI223)+DD133  76300000
               4*(YI134-YI132)+DD132*(YI131-YI133)+DD123*(YI124-YI122)+DD122*   76400000
               5(YI121-YI123))/DELZZ)+DD223*YI213/DELRR+DD232*YI231/DELZZ       76500000
005725          YDE = ((((DD223-G)/DELRR+DD232/DELZZ)/RESC8+F1)+F2)             76600000
005735          TEMPY(I,M,N) = ((((Y2RD+G*((YI232-YI222)+(YI133-YI123)+(YI132-  76700000
               1YI122)-YI223)/DELRR)/RESC8+UCTI(I,M,N,WI1,WI2)*DAM)-0.25*S*(Y*  76800000
               2((YI232-YI222)+(YI133-YI123)+(YI132-YI122)-YI223)/DELR+Z*((YI223-  76900000
               3YI222)+(YI133-YI132)+(YI123-YI122)-YI232)/DELZ))-F2*((YI232-YI132)  77000000
               4+(YI223-YI123)+(YI222-YI122)-YI133))/YDE                        77100000
006016          IF(TEMPY(I,M,N)-AMIN) 555, 555, 556                             77200000
006022      555 TEMPY(I,M,N) = C.0                                              77300000
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006027      555 IF(TEMPY(I,M,N)-1.0) 560, 560, 558                          77400000
005036      558 TEMPY(I,M,N) = 1.0                                          77500000
006044      560 CONTINUE                                                    77600000
          C-----                                                            77700000
          C     CALCULATE MASS FRACTION FROM BOUNDARY EQUATIONS.            77800000
          C-----                                                            77900000
006054          DO 570 I = 1, NI                                            78000000
006055          DO 570 N = 2, N7                                            78100000
006056          TEMPY(I,1,N) = TEMPY(I,2,N)                                 78200000
006065      570 CONTINUE                                                    78300000
          C-----                                                            78400000
          C     COMPARE CALCULATED AND GUESS VALUES.                        78500000
          C     IF THE DIFFERENCE IS GREATER THAN THE ALLOWED ERROR.        78600000
          C     SET CALCULATED VALUES AS NEW GUESS VALUES AND REPEAT CALCULATIONS.  78700000
          C     IF THE DIFFERENCE IS LESS THAN THE ALLOWED ERROR. PRINT CALCULATED  78800000
          C     VALUES.                                                     78900000
          C-----                                                            79000000
006072          ADT = 0.0                                                   79100000
006073          ADR = 0.0                                                   79200000
006074          AD7 = 0.0                                                   79300000
006075          ADY = 0.0                                                   79400000
006076          ADS = 0.0                                                   79500000
006077          SUMT = 0.0                                                  79600000
006100          SUMR = 0.0                                                  79700000
006101          SUM7 = 0.0                                                  79800000
006102          SUMY = 0.0                                                  79900000
006103          SUMS = 0.0                                                  80000000
006104          K = 1                                                       80100000
006105          DO 675 MS = 1, NWS1                                         80200000
006106          DO 675 N = 2, N7                                            80300000
006107          AD = ABS(TEMPS(MS,N)-TS(2,MS,N))*TRA                        80400000
006117          ADS = ADS + AD                                              80500000
006121          SUMS = SUMS + TS(2,MS,N)                                    80600000
006126          IF(AD-AMAX) 675, 675, 715                                   80700000
006130      675 CONTINUE                                                    80800000
006135          IF(ADS-AE*ABS(SUMS)) 680, 680, 715                          80900000
006142      680 K = 2                                                       81000000
006143          DO 685 N = 2, N7                                            81100000
006145          DO 685 M = 2, NW                                            81200000
006146          AD = ABS(TEMPR(M,N)-VR(2,M,N))                              81300000
006155          ADR = ADR + AD                                              81400000
006157          SUMR = SUMR + ABS(VR(2,M,N))                                81500000
006165          IF(AD-AMAX) 685, 685, 715                                   81600000
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006170      685 CONTINUE                                                    81700000
006175          IF(ADR-AE*SUMR) 690, 690, 715                               81800000
006201      690 K = 3                                                       81900000
006202          DO 695 N = 2, NZ                                            82000000
006204          DO 695 M = 2, NM1                                           82100000
006205          AD = ABS(TEMPZ(M,N)-VZ(2,M,N))                              82200000
006214          ADZ = ADZ + AD                                              82300000
006216          SUMZ = SUMZ + ABS(VZ(2,M,N))                                82400000
006224          IF(AD-AMAX) 695, 695, 715                                   82500000
006227      695 CONTINUE                                                    82600000
006234          IF(ADZ-AE*SUMZ) 700, 700, 715                               82700000
006240      700 DO 710 N = 2, NZ                                            82800000
006242          DO 710 M = 1, NM1                                           82900000
006243          AD = ABS(TEMPT(M,N)-T(2,M,N))                               83000000
006252          ADT = ADT + AD                                              83100000
006254          SUMT = SUMT + T(2,M,N)                                      83200000
006261          K = 4                                                       83300000
006262          IF(AD-AMAX) 705, 705, 715                                   83400000
006264      705 DO 710 I = 1, NI1                                           83500000
006266          K = K + 1                                                   83600000
006270          AD = ABS(TEMPY(I,M,N)-YI2(I,M,N))                           83700000
006301          ADY = ADY + AD                                              83800000
006302          SUMY = SUMY + YI2(I,M,N)                                    83900000
006307          IF(AD-AMAX) 710, 710, 715                                   84000000
006311      710 CONTINUE                                                    84100000
006321          IF(ADT-AE*ABS(SUMT)) 712, 712, 715                          84200000
006325      712 IF(ADY-AE*ABS(SUMY)) 714, 714, 715                          84300000
006332      714 GO TO 848                                                   84400000
006333      715 IF (NIT-IT) 720, 720, 730                                   84500000
        C-----                                                              84600000
        C       PRINT ALL CALCULATED DEPENDENT VARIABLES AT END OF ITERATIONS. 84700000
        C-----                                                              84800000
006336      720 CALL FORM1(3,YI2)                                           84900000
        C-----                                                              85000000
        C       TERMINATE PROGRAM AT END OF NIT ITERATIONS.                 85100000
        C-----                                                              85200000
006340          WRITE(6,725) IT, K, M, N, MS, AD                            85300000
006360      725 FORMAT(1H1,//5X,28HTERMINATE PROGRAM AT END OF ,I2,11H ITERATIONS/ 85400000
           1 6X,41H---------------------------------------- ///20X,4HK = ,I2, 85500000
           2 20X,4HM = ,I2,20X,4HN = ,I2,20X,5HMS = ,I2//20X,5HAD = ,E12.4) 85600000
006360          STOP3                                                       85700000
        C-----                                                              85800000
        C       ACCELERATING CONVERGENCE PROCEDURE= AITKEN*S DEL-SQUARE METHOD. 85900000
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```
      C      IT = 1, CONTINUE ITERATION.
      C      IT = 2, STORE VALUES FOR ALL THE DELT-A.
      C      IT = 3, STORE VALUES FOR ALL THE DELT-B.
      C-----
006362   730 IF(IT-2) 820, 735, 765
      C-----
      C      STORE VALUES FOR ALL THE DELT-A.
      C-----
006365   735 DO 764 N = 2, NZ
006367       DO 740 M = 1, NW1
006370       DELA = T(2,M,N)-TEMT(M,N)
006377       DELB = TEMPT(M,N)-T(2,M,N)
006405       IF(DELB-DELA) 738, 736, 738
006407   736 DELTTA(M,N) = TEMPT(M,N)
006415       GO TO 740
006415   738 DELTTA(M,N) = TEMT(M,N)-DELA*DELA/(DELB-DELA)
006427   740 CONTINUE
006432       DO 746 M = 2, NW
006433       DELA = VR(2,M,N)-TEMR(M,N)
006442       DELB = TEMPR(M,N)-VR(2,M,N)
006450       IF(DELB-DELA) 744, 742, 744
006452   742 DELTRA(M,N) = TEMPR(M,N)
006460       GO TO 746
006460   744 DELTRA(M,N) = TEMR(M,N)-DELA*DELA/(DELB-DELA)
006472       IF(ABS(DELTRA(M,N))-AMIN) 745, 745, 746
006475   745 DELTRA(M,N) = 0.0
006501   746 CONTINUE
006504       DO 752 M = 2, NW1
006505       DELA = VZ(2,M,N)-TEMZ(M,N)
006514       DELB = TEMPZ(M,N)-VZ(2,M,N)
006522       IF(DELB-DELA) 750, 748, 750
006524   748 DELTZA(M,N) = TEMPZ(M,N)
006532       GO TO 752
006532   750 DELTZA(M,N) = TEMZ(M,N)-DELA*DELA/(DELB-DELA)
006544   752 CONTINUE
006547       DO 758 M = 1, NW1
006550       DO 758 I = 1, NI
006551       DELA = YI2(I,M,N)-TEMY(I,M,N)
006562       DELB = TEMPY(I,M,N)-YI2(I,M,N)
006565       IF(DELB-DELA) 756, 754, 756
006567   754 DELTYA(I,M,N) = TEMPY(I,M,N)
006577       GO TO 758
006600   756 DELTYA(I,M,N) = TEMY(I,M,N)-DELA*DELA/(DELB-DELA)
```

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006614          IF(DELTYA(I,M,N)-AMIN) 757, 757, 758
006620      757 DELTYA(I,M,N) = C.0
006625      758 CONTINUE
006632          DO 764 MS = 1, NKS1
006634          DELA = TS(2,MS,N)-TEMS(MS,N)
006642          DELB = TEMPS(MS,N)-TS(2,MS,N)
006650          IF(DELB-DELA) 762, 760, 762
006652      760 DELTSA(MS,N) = TEMPS(MS,N)
006657          GO TO 764
006660      762 DELTSA(MS,N) = TEMS(MS,N)-DELA*DELA/(DELB-DELA)
006671      764 CONTINUE
006676          GO TO 820
        C-----
        C       STORE VALUES FOR ALL THE DELT-B.
        C-----
006677      765 DO 794 N = 2, NZ
006701          DO 770 M = 1, NK1
006702          DELA = T(2,M,N)-TEMT(M,N)
006711          DELB = TEMPT(M,N)-T(2,M,N)
006717          IF(DELB-DELA) 768, 766, 768
006721      766 DELTTB(M,N) = TEMPT(M,N)
006727          GO TO 770
006727      768 DELTTB(M,N) = TEMT(M,N)-DELA*DELA/(DELB-DELA)
006741      770 CONTINUE
006744          DO 776 M = 2, NK
006745          DELA = VR(2,M,N)-TEMR(M,N)
006754          DELB = TEMPR(M,N)-VR(2,M,N)
006762          IF(DELB-DELA) 774, 772, 774
006764      772 DELTRB(M,N) = TEMPR(M,N)
006772          GO TO 776
006772      774 DELTRB(M,N) = TEMR(M,N)-DELA*DELA/(DELB-DELA)
007004          IF(ABS(DELTRB(M,N))-AMIN) 775, 775, 776
007007      775 DELTRB(M,N) = C.0
007013      776 CONTINUE
007016          DO 782 M = 2, NK1
007017          DELA = VZ(2,M,N)-TEMZ(M,N)
007026          DELB = TEMPZ(M,N)-VZ(2,M,N)
007034          IF(DELB-DELA) 780, 778, 780
007036      778 DELTZB(M,N) = TEMPZ(M,N)
007044          GO TO 782
007044      780 DELTZB(M,N) = TEMZ(M,N)-DELA*DELA/(DELB-DELA)
007056      782 CONTINUE
007061          DO 789 M = 1, NK1
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007062          DO 789 I = 1, NI                                                94600000
007063          DELA = YI2(I,M,N)-TEMY(I,M,N)                                   94700000
007074          DELB = TEMPY(I,M,N)-YI2(I,M,N)                                  94800000
007077          IF(DELB-DELA) 786, 784, 786                                     94900000
007101      784 DELTYB(I,M,N) = TEMPY(I,M,N)                                    95000000
007111          GO TO 787                                                       95100000
007112      786 DELTYB(I,M,N) = TEMY(I,M,N)-DELA*DELA/(DELB-DELA)               95200000
007126      787 IF(DELTYB(I,M,N)-AMIN) 788, 788, 789                            95300000
007135      788 DELTYB(I,M,N) = 0.0                                             95400000
007142      789 CONTINUE                                                        95500000
007147          DO 794 MS = 1, NMS1                                             95600000
007151          DELA = TS(2,MS,N)-TEMS(MS,N)                                    95700000
007157          DELB = TEMPS(MS,N)-TS(2,MS,N)                                   95800000
007165          IF(DELB-DELA) 792, 790, 792                                     95900000
007167      790 DELTSB(MS,N) = TEMPS(MS,N)                                      96000000
007174          GO TO 794                                                       96100000
007175      792 DELTSB(MS,N) = TEMS(MS,N)-DELA*DELA/(DELB-DELA)                 96200000
007206      794 CONTINUE                                                        96300000
        C-----                                                                  96400000
        C       TEST FOR CONVERGENCE.                                           96500000
        C-----                                                                  96600000
007213          ADT = 0.0                                                       96700000
007214          ADR = 0.0                                                       96800000
007215          ADZ = 0.0                                                       96900000
007216          ADY = 0.0                                                       97000000
007217          ADS = 0.0                                                       97100000
007220          SUMT = 0.0                                                      97200000
007221          SUMR = 0.0                                                      97300000
007222          SUMZ = 0.0                                                      97400000
007223          SUMY = 0.0                                                      97500000
007224          SUMS = 0.0                                                      97600000
007225          K = 1                                                           97700000
007226          DO 799 N = 2, NZ                                                97800000
007227          IF(TSO*DELTSA(1,N)-TSC) 795, 796, 796                           97900000
007234      795 DELTSA(1,N) = TSC/TSO                                           98000000
007240      796 IF(TSO*DELTSB(1,N)-TSC) 797, 798, 798                           98100000
007245      797 DELTSB(1,N) = TSC/TSO                                           98200000
007251      798 DO 799 MS = 1, NMS1                                             98300000
007253          AD = ABS(DELTSB(MS,N)-DELTSA(MS,N))*TRA                         98400000
007262          ADS = ADS + AD                                                  98500000
007264          SUMS = SUMS + DELTSA(MS,N)                                      98600000
007270          IF(AD-AMAX) 799, 799, 810                                       98700000
007272      799 CONTINUE                                                        98800000
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```
007277          IF(ADS-AE*ABS(SUMS)) 800, 800, 810                      98900000
007304      800 K = 2                                                   99000000
007305          DO 801 N = 2, NZ                                        99100000
007307          DO 801 M = 2, Nw                                        99200000
007310          AD = ABS(DELTRB(M,N)-DELTRA(M,N))                       99300000
007317          ADR = ADR + AD                                          99400000
007321          SUMR = SUMR + ABS(DELTRA(M,N))                          99500000
007325          IF(AD-AMAX) 801, 801, 810                               99600000
007327      801 CONTINUE                                                99700000
007334          IF(ADR-AE*SUMR) 802, 802, 810                           99800000
007340      802 K =3                                                    99900000
007341          DO 803 N = 2, NZ                                       100000000
007343          DO 803 M = 2, Nw1                                      100100000
007344          AD = ABS(DELTZB(M,N)-DELTZA(M,N))                      100200000
007353          ADZ = ADZ + AD                                         100300000
007355          SUMZ = SUMZ + ABS(DELTZA(M,N))                         100400000
007361          IF(AD-AMAX) 803, 803, 810                              100500000
007363      803 CONTINUE                                               100600000
007370          IF(ADZ-AE*SUMZ) 804, 804, 810                          100700000
007374      804 DO 806 N = 2, NZ                                       100800000
007376          DO 806 M = 1, Nw1                                      100900000
007377          AD = ABS(DELTTB(M,N)-DELTTA(M,N))                      101000000
007406          ADT = ADT + AD                                         101100000
007410          SUMT = SUMT + DELTTA(M,N)                              101200000
007413          K = 4                                                  101300000
007414          IF(AD-AMAX) 805, 805, 810                              101400000
007416      805 DO 806 I = 1, NTI                                      101500000
007420          K = K + 1                                              101600000
007422          AD = ABS(DELTYB(I,M,N)-DELTYA(I,M,N))                  101700000
007433          ADY = ADY + AD                                         101800000
007434          SUMY = SUMY + DELTYA(I,M,N)                            101900000
007441          IF(AD-AMAX) 806, 806, 810                              102000000
007443      806 CONTINUE                                               102100000
007453          IF(ADT-AE*ABS(SUMT)) 807, 807, 810                     102200000
007457      807 IF(ADY-AE*ABS(SUMY)) 808, 808, 810                     102300000
007464      808 GO TO 834                                              102400000
        C-----                                                         102500000
        C       RESET VALUES FOR ALL THE DELT-A.                       102600000
        C-----                                                         102700000
007465      810 DO 819 N = 2, NZ                                       102800000
007467          DO 812 M = 1, Nw1                                      102900000
007470      812 DELTTA(M,N) = DELTTB(M,N)                              103000000
007501          DO 814 M = 2, Nw                                       103100000
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007502      814 DELTRA(M,N) = DELTRB(M,N)                                   103200000
007513          DO 816 M = 2, NW1                                           103300000
007514      816 DELTZA(M,N) =DELTZB(M,N)                                    103400000
007525          DO 819 I = 1, NI                                            103500000
007526          DO 818 M = 1, NW1                                           103600000
007527      818 DELTYA(I,M,N) = DELTYB(I,M,N)                               103700000
007546          DO 819 MS = 1, NWS1                                         103800000
007547      819 DELTSA(MS,N) = DELTSB(MS,N)                                 103900000
          C-----                                                            104000000
          C     SET NEW GUESS VALUES FOR ALL DEPENDENT VARIABLES.           104100000
          C-----                                                            104200000
007562      820 DO 832 N = 2, NZ                                            104300000
007564          DO 822 M = 1, NW                                            104400000
007565          TEMT(M,N) = T(2,M,N)                                        104500000
007573      822 T(2,M,N) = 0.1*TEMPT(M,N)+0.9*T(2,M,N)                      104600000
007606          DO 824 M = 2, NW                                            104700000
007607          TEMR(M,N) = VR(2,M,N)                                       104800000
007615      824 VR(2,M,N) = 0.1*TEMPR(M,N)+0.9*VR(2,M,N)                    104900000
007630          DO 826 M = 2, NW1                                           105000000
007631          TEMZ(M,N) = VZ(2,M,N)                                       105100000
007637      826 VZ(2,M,N) =0.1*TEMPZ(M,N)+0.9*VZ(2,M,N)                     105200000
007652          DO 828 M = 1, NW1                                           105300000
007653          DO 828 I = 1, NI                                            105400000
007654          TEMY(I,M,N) = YI2(I,M,N)                                    105500000
007664      828 YI2(I,M,N) =0.1*TEMPY(I,M,N)+0.9*YI2(I,M,N)                 105600000
007676          DO 832 MS = 1, NWS1                                         105700000
007677          TEMS(MS,N) = TS(2,MS,N)                                     105800000
007704      832 TS(2,MS,N) =0.1*TEMPS(MS,N)+0.9*TS(2,MS,N)                  105900000
          C-----                                                            106000000
          C     REPEAT ITERATION.                                           106100000
          C-----                                                            106200000
007720          GO TO 125                                                   106300000
          C-----                                                            106400000
          C     CONVERGENCE - SET ALL DELT-B AS TEMP-.                      106500000
          C-----                                                            106600000
007721      834 DO 847 N = 2, NZ                                            106700000
007723          DO 836 M = 1, NW1                                           106800000
007724      835 TEMPT(M,N) = DELTTB(M,N)                                    106900000
007735          DO 838 M = 2, NW                                            107000000
007736      838 TEMPR(M,N) = DELTRB(M,N)                                    107100000
007747          DO 840 M = 2, NW1                                           107200000
007750      840 TEMPZ(M,N) = DELTZB(M,N)                                    107300000
007761          DO 842 I = 1, NI                                            107400000
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007762          DO 842 M = 1, NW1                                       107500000
007763      842 TEMPY(I,M,N) = DELTYB(I,M,N)                            107600000
010002          DO 846 MS = 1, NWS1                                     107700000
010003      846 TEMPS(MS,N) = DELTSB(MS,N)                              107800000
010014      847 TEMPT(NW,N) = TRA*TEMPS(1,N)                            107900000
        C-----                                                          108000000
        C       CALCULATE VALUE FOR THE TOTAL TIME.                     108100000
        C-----                                                          108200000
010024      849 L1 = L -1                                               108300000
010026          TIME = L1*ADELT + TIMEI                                 108400000
        C-----                                                          108500000
        C       PRINT VALUES OF DEPENDENT VARIABLES AT TIME STEPS EQUAL TO A  108600000
        C       MULTIPLE OF LL.                                         108700000
        C-----                                                          108800000
010031          IF(MOD(L1,LL)-0) 850, 849, 850                          108900000
010036      849 CALL FORM1(3,YI2)                                       109000000
        C-----                                                          109100000
        C       INTERPOLATE VALUES FOR ALL VARIABLES AT NEXT TIME STEP. 109200000
        C-----                                                          109300000
010040      850 DO 880 N = 2, NZ                                        109400000
010042          DO 855 M = 2, NW                                        109500000
010043      855 VR(2,M,N) = 2.0*(TEMPR(M,N))-VR(1,M,N)                  109600000
010062          DO 860 M = 2, NW1                                       109700000
010064      860 VZ(2,M,N) = 2.0*(TEMPZ(M,N))-VZ(1,M,N)                  109800000
010103          DO 870 M = 1, NW1                                       109900000
010105          T(2,M,N) = 2.0*(TEMPT(M,N))-T(1,M,N)                    110000000
010120          DO 870 I = 1, NI                                        110100000
010122      870 YI2(I,M,N) = 2.0*(TEMPY(I,M,N))-YI1(I,M,N)              110200000
010143          DO 875 MS = 1, NWS1                                     110300000
010145      875 TS(2,MS,N) = 2.0*TEMPS(MS,N)-TS(1,MS,N)                 110400000
010163      880 T(2,NW,N) = TRA*TS(2,1,N)                               110500000
        C-----                                                          110600000
        C       SET VALUES FOR PREVIOUS KNOWN TIME STEP.                110700000
        C-----                                                          110800000
010174          DO 930 N = 2, NZ                                        110900000
010175          DO 900 M = 2, NW                                        111000000
010176          DEN(1,M,N) = DEN(2,M,N)                                 111100000
010205      900 VR(1,M,N) = TEMPR(M,N)                                  111200000
010213          DO 910 M = 2, NW1                                       111300000
010215      910 VZ(1,M,N) = TEMPZ(M,N)                                  111400000
010227          DO 920 M = 1, NW1                                       111500000
010230          T(1,M,N) = TEMPT(M,N)                                   111600000
010236          DO 920 I = 1, NI                                        111700000
```

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010240      92) YI1(I,M,N) = TEMPY(I,M,N)                                    111800000
010257          DO 925 MS = 1, NWSI                                          111900000
010260     925 TS(1,MS,N) = TEMPS(MS,N)                                      112000000
010271     930 T(1,NW,N) = TRA*TS(1,1,N)                                     112100000
         C-----                                                              112200000
         C      SET INITIAL VALUES OF NON-DIMENSIONALIZED FUNCTIONS FOR NEXT TIME  112300000
         C      STEP.                                                        112400000
         C-----                                                              112500000
010302          CALL SUB1(1,YI1)                                             112600000
010304     990 CONTINUE                                                      112700000
         C-----                                                              112800000
         C      TERMINATE PROGRAM AT END OF NT TIME STEPS.                   112900000
         C-----                                                              113000000
010307          WRITE(6,999) NT                                              113100000
010314     999 FORMAT(//5X,28HTERMINATE PROGRAM AT END OF ,I4,12H TIME STEPS.)  113200000
         C-----                                                              113300000
         C      STORE DATA ON TAPE.                                          113400000
         C-----                                                              113500000
010314          REWIND 8                                                     113600000
010316          DO 1100 I = 1, NT                                            113700000
010320          WRITE(8) ((YI1(I,M,N), N = 1, NZ), M = 1, NW)                113800000
010340          WRITE(8) ((YI2(I,M,N), N = 1, NZ), M = 1, NW)                113900000
010360     110) CONTINUE                                                     114000000
010363          DO 1200 L = 1, 2                                             114100000
010364          WRITE(8) ((DEN(L,M,N), N =1, NZ), M = 1,NW)                  114200000
010404          WRITE(8) (( VR(L,M,N), N =1, NZ), M = 1,NW)                  114300000
010424          WRITE(8) (( VZ(L,M,N), N =1, NZ), M = 1,NW)                  114400000
010444          WRITE(8) ((  T(L,M,N), N =1, NZ), M = 1,NW)                  114500000
010464          WRITE(8) ((  P(L,M,N), N =1, NZ), M = 1,NW)                  114600000
010504          WRITE(8) ((   TS(L,MS,N), N = 1, NZ), MS = 1, NWS)           114700000
010523          WRITE(8) (( DENS(L,MS,N), N = 1, NZ), MS = 1, NWS)           114800000
010542          WRITE(8) ((ALAMS(L,MS,N), N = 1, NZ), MS = 1, NWS)           114900000
010561          WRITE(8) ((   CS(L,MS,N), N = 1, NZ), MS = 1, NWS)           115000000
010600     120) CONTINUE                                                     115100000
010602          WRITE(8) TIME, ((RR(L,N), N = 1, NZ), L = 1, 2), (R(M), M =1, NW)  115200000
         C-----                                                              115300000
         C      PUNCH OUT VALUES OF ALL DEPENDENT VARIABLES FOR P OTTING.    115400000
         C-----                                                              115500000
010630          DO 3000 N = 4, NZ, 3                                         115600000
010632          PUNCH 2100, (DEN(1,M,N), M = 1, NW), TIME, N                 115700000
010651     210) FORMAT(5G12.5/5G12.5/5G12.5/6G12.5,6X,I2)                    115800000
010651          PUNCH 2100, ( VR(1,M,N), M = 1, NW), TIME, N                 115900000
010671          PUNCH 2100, ( VZ(1,M,N), M = 1, NW), TIME, N                 116000000
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010711          PUNCH 2100, (  T(1,M,N), M = 1, NW), TIME, N                    116100000
010731          DO 2300 I = 1, NT                                               116200000
010733     2300 PUNCH 2100, (YI1(I,M,N), M = 1, NW), TIME, N                    116300000
010756          PUNCH 2400, ( TS(1,M,N), M = 1, NWS), TIME, N                   116400000
010775     2400 FORMAT(5G12.5/5G12.5/6G12.5,6X,I2)                              116500000
010775     3000 CONTINUE                                                        116600000
011000          STOP                                                            116700000
011002          END                                                             116800000
          C                                                                     116900000
```

```
                SUBROUTINE VEL(U,NM,NN,NNR,DEL1,DEL2)                   117000000
        C-----                                                          117100000
        C       THIS PROGRAM CALCULATES AXIAL VELOCITY VALUES AT ALL GRID POINTS  117200000
        C       BASED ON THE 1/7 POWER VELOCITY PROFILE FOR TURBULENT FLOW.  117300000
        C-----                                                          117400000
000011          DIMENSION U(2,20,10)                                    117500000
000011          COMMON/FUN/DELR,DELZ,R(20)                              117600000
000011          NM1 = NM - 1                                            117700000
000013          X = 1.0/7.0                                             117800000
000015          DO 40 L = 1, 2                                          117900000
000015          DO 40 N = 1, NN                                         118000000
000017          U(L,NM,N) = 0.0                                         118100000
000023          DO 40 M = 1, NM1                                        118200000
000025          IF(M-NNR) 10, 20, 20                                    118300000
000027       10 R(M) = (M-1)*DEL1                                       118400000
000034          GO TO 40                                                118500000
000034       20 R(M) = (M+1-NNR)*DEL2+(NNR-2)*DEL1                      118600000
000045       40 U(L,M,N) = (1.0-R(M))**X                                118700000
000070          RETURN                                                  118800000
000071          END                                                     118900000
        C                                                               119000000
```

```
                SUBROUTINE SUB1(J,UYI)
          C-----
          C     THIS PROGRAM CALCULATES ALL THE NON-DIMENSIONALIZED FUNCTIONS AT
          C     ANY TIME STEP.
          C-----
000005          DIMENSION UYI(3,20,10),UDI(3,20,10),UWI(3,20,10),UCPI(3,20,10),
               1UHI(3,20,10)
000005          COMMON RO,AMUO,DO,WO,ALAMO,CPO,DENSO,ALAMSO,CSO,FRO,FC,
               1AMI(3),CAI(3),CBI(3),CCI(3),HSL(3),HIO(3),CP(2,20,10),HLG(3),
               2P(2,20,10), AMU(2,20,10), ALAM(2,20,10), HSGI(2,3,10),TBP(3),
               3DENS(2,15,10), CS(2,15,10), RR(2,10), ALAMS(2,15,10)
000005          COMMON/FORM/NW,NWS,NZ,NI,ANU1,ANU2,ANU3,CF,TC,TSC,FLL,FLU,L,IT,SF,
               1RA1,RA2,VO,TO,DENO,TSO,TIME,DEN(2,20,10),T(2,20,10),TS(2,15,10)
000005          COMMON/SPEC/DI1(3,20,10),DI2(3,20,10),WI1(3,20,10),WI2(3,20,10),
               1CPI1(3,20,10),CPI2(3,20,10),HI1(3,20,10),HI2(3,20,10)
          C-----
          C     CALCULATE RATE OF PRODUCTION OF SPECIES,I.
          C-----
          C     F IS THE THEORETICAL FUEL-OXIDIZER RATIO.
          C-----
000005          F = ANU2*AMI(2)/(ANU1*AMI(1))
000010          RCO = 1.0
000012          ROF = 2.0
000013          AN = 6.023E+23
000015          CF1 = 1.1608524E+09
000016          CF2 = 1.6018222E-02
000020          CF3 = 905.98827
000021          DO 20 M = 1, NW
000023          DO 20 N = 1, NZ
000024          IF(UYI(1,M,N)-0.0) 10,10,1
000031        1 IF(UYI(2,M,N) - .0) 10, 10, 5
000037        5 IF(T(J,M,N)-TC/TC) 10, 6, 6
000047        6 IF(UYI(2,M,N)/UYI(1,M,N) - FLL*F) 10, 7, 7
000062        7 IF(FLU*F-UYI(2,M,N)/UYI(1,M,N)) 10, 15, 15
000075       10 UWI(1,M,N) = 0.0
000102          UWI(2,M,N) = 0.0
000106          UWI(3,M,N) = 0.0
000112          GO TO 20
000113       15 Z12 = ((RA1+RA2)**2.0)*1.0E-16
000121          Z12 = Z12*SQRT(CF1*TO*T(J,M,N)*(AMI(1)+AMI(2))/(AMI(1)*AMI(2)))
000141          A1 = DENO*DEN(J,M,N)*UYI(1,M,N)/AMI(1)
000153          A2 = DENO*DEN(J,M,N)*UYI(2,M,N)/AMI(2)
```

```
000165          AN1 = CF2*A1                                                    123300000
000167          AN2 = CF2*A2                                                    123400000
000170          A1 = AN1**RCG                                                   123500000
000174          A2 = AN2**RCF                                                   123600000
000200          AK = AN*712*SF*EXP(-CE*CF3/T(J,M,N)/TO)                         123700000
000217          CA = AK*A1*A2/(WO*CF2)                                          123800000
000223          UNI(1,M,N) = -AMI(1)*ANU1*CA                                    123900000
000232          UNI(2,M,N) = -AMI(2)*ANU2*CA                                    124000000
000240          UNI(3,M,N) =  AMI(3)*ANU3*CA                                    124100000
000245       20 CONTINUE                                                        124200000
000252          DO 30 I = 1, NI                                                 124300000
000254          DO 30 M = 1, NW                                                 124400000
000255          DO 30 N = 1, NZ                                                 124500000
        C-----                                                                  124600000
        C       CALCULATE DIFFUSION COEFFICIENT OF SPECIES, I.                  124700000
        C-----                                                                  124800000
000256          DDI(I,M,N) = 20.                                                124900000
        C-----                                                                  125000000
        C       CALCULATE SPECIFIC HEAT PER UNIT MASS OF SPECIES, I, AT CONSTANT 125100000
        C       PRESSURE.                                                       125200000
        C-----                                                                  125300000
000264          UCPI(I,M,N)=(CAI(I)+TO*T(J,M,N)*(CBI(I)+TO*T(J,M,N)*CCI(I)))/CPO 125400000
        C                                                                       125500000
        C       CALCULATE ENTHALPY PER UNIT MASS OF SPECIES, I.                 125600000
        C                                                                       125700000
000304          FHI = T(J,M,N)*(CAI(I)+TO*T(J,M,N)*(CBI(I)/2.0+TO*T(J,M,N)*CCI(I) 125800000
               1/3.0))-536.4*(CAI(I)+536.4*(CBI(I)/2.0+536.4*CCI(I)/3.0))/TO    125900000
000334          UHI(I,M,N) =  (FHI+(HIO(I)+HSL(I))/TO)/CPO                      126000000
000347          IF(T(J,M,N)*TO-TRP(I)) 30, 30, 28                               126100000
000356       28 UHI(I,M,N) = UHI(I,M,N) + HLG(I)/(TO*CPO)                       126200000
000367       30 CONTINUE                                                        126300000
000377          DO 60 M = 1, NW                                                 126400000
000400          DO 60 N = 1, NZ                                                 126500000
        C-----                                                                  126600000
        C       CALCULATE VISCOSITY OF GAS MIXTURE.                             126700000
        C-----                                                                  126800000
000401          AMU(J,M,N) = 20.                                                126900000
        C-----                                                                  127000000
        C       CALCULATE THERMAL CONDUCTIVITY OF GAS MIXTURE.                  127100000
        C-----                                                                  127200000
000406          ALAM(J,M,N) = 20.                                               127300000
        C-----                                                                  127400000
        C       CALCULATE SPECIFIC HEAT PER UNIT MASS OF GAS MIXTURE AT CONSTANT 127500000
```

```
C      PRESSURE.
C-----
000413        CP(J,M,N) = 0.0
000417        DO 50 I = 1, NI
000420     50 CP(J,M,N) = CP(J,M,N) + UYI(I,M,N)*UCPI(I,M,N)
000442     60 CONTINUE
000447        IF(J-1) 62,62,64
000451     62 DO 63 I = 1, NI
000453        DO 63 M = 1, NW
000454        DO 63 N = 1, NZ
000455        DI1(I,M,N) = UDI(I,M,N)
000466        WI1(I,M,N) = UWI(I,M,N)
000471        CPI1(I,M,N) = UCPI(I,M,N)
000475        HI1(I,M,N) = UHI(I,M,N)
000500     63 CONTINUE
000507        GO TO 68
000510     64 DO 65 I = 1, NI
000512        DO 65 M = 1, NW
000513        DO 65 N = 1, NZ
000514        DI2(I,M,N) = UDI(I,M,N)
000525        WI2(I,M,N) = UWI(I,M,N)
000530        CPI2(I,M,N) = UCPI(I,M,N)
000534        HI2(I,M,N) = UHI(I,M,N)
000537     65 CONTINUE
C-----
C      CALCULATE HEAT OF SUBLIMATION OF SPECIES, I, IN SOLID FUEL.
C-----
000546     68 DO 90 N = 1, NZ
000550        HSGI(J,1,N) = 0.0
000553        HSGI(J,3,N) = 0.0
000556        IF(TS(J,1,N)-TSC/TSO) 70, 80, 80
000564     70 HSGI(J,2,N) = 0.0
000570        GO TO 90
000571     80 HSGI(J,2,N) = (HSL(2)+HLG(2))/(CSO*TSO)
000601     90 CONTINUE
C-----
C      IF TIME = ZERO, CONTINUE CALCULATIONS, OTHERWISE, RETURN.
C-----
000604        IF(TIME-0.0) 150, 95, 150
000606     95 DO 100 MS = 1, NWS
000610        DO 100 N = 1, NZ
C-----
C      CALCULATE DENSITY OF SOLID FUEL.
```

```
        C-----
000611        EMS(J,MS,N) = 1.0
        C-----
        C     CALCULATE THERMAL CONDUCTIVITY OF SOLID FUEL.
        C-----
000616        ALAMS(J,MS,N) = 1.0
        C-----
        C     CALCULATE SPECIFIC HEAT PER UNIT MASS OF SOLID FUEL.
        C-----
000623        CS(J,MS,N) = 1.0
000626    100 CONTINUE
        C-----
        C     CALCULATE REGRESSION RATE OF FUEL.
        C-----
000633        RR(J,1) = 0.0
000635        DO 130 N = 2, N7
000636        RR(J,N) = 1.0
000642    130 CONTINUE
000644    150 RETURN
000645        END
        C
```

```
                SUBROUTINE FORM1(J,UYI)
          C-----
          C     THIS PROGRAM PRINTS OUT INPUT DATA OR CALCULATED VALUES OF
          C     DEPENDENT VARIABLES IN THEIR APPROPRIATE DIMENSIONS.
          C     J = 1,  INPUT DATA AT TIME STEP = 1.
          C     J = 2,  INPUT DATA AT TIME STEP = 2.
          C     J = 3, CALCULATED VALUES.
          C-----
000005          DIMENSION UYI(3,20,10),CONVT(10)
          C-----
000005          COMMON/CAL/VR(2,20,10),VZ(2,20,10),TEMPR(20,10),TEMPZ(20,10),
               1TEMPT(20,10),TEMPS(15,10),TEMPY(3,20,10)
          C-----
000005          COMMON/FORM/NW,NWS,NZ,NI,ANU1,ANU2,ANU3,CF,TC,TSC,FLL,FLU,L,IT,SF,
               1RA1,RA2,VC,TC,DENO,TSO,TIME,DEN(2,20,10),T(2,20,10),TS(2,15,10)
          C-----
000005          IF(J -2) 5, 5, 829
          C-----
          C     PRINT OUT INPUT DATA.
          C-----
000007        5 WRITE(6,10) J, TIME
000017       10 FORMAT (1H1,2X,19HINPUT= TIME STEP = ,I2,70X,7HTIME = ,G11.4,
               15H SEC./2X,23H----------------------- ,69X,4H---- )
000017          WRITE(6,11)
000023       11 FORMAT (/50X,26HDENSITY AT GRID POINT(M,N)/50X,26H----------------
               1---------- )
000023          WRITE(6,15) (N, N = 1, NZ)
000035       15 FORMAT(//2X,2HN=,2X,10(I6,6X)/2X,2H M)
000035          DO 20 M = 1, NW
000040          DO 18 N = 1, NZ
000041       18 CONVT(N) = DENO*DEN(J,M,N)
000053       20 WRITE(6,21) M, (CONVT(N), N = 1, NZ)
000074       21 FORMAT (/2X,I2,2X,10G12.5)
000074          WRITE(6,25)
000100       25 FORMAT(////20X,4HNOTE,10X,36HM IS GRID NUMBER IN RADIAL DIRECTION/
               120X,4H----,10X,35HN IS GRID NUMBER IN AXIAL DIRECTION)
000100          WRITE(6,10)J, TIME
000111          WRITE(6,31)
000115       31 FORMAT(/50X,29HR-VELOCITY AT GRID POINT(M,N)/50X,29H--------------
               1--------------- )
000115          WRITE(6,15) (N, N = 1, NZ)
000127          DO 40 M = 1, NW
```

```
000132          DO 35 N = 1, NZ                                                 138200000
000133       35 CONVT(N) = VO*VR(J,M,N)                                         138300000
000145       40 WRITE(6,21) M, (CONVT(N), N = 1, NZ)                            138400000
000166          WRITE(6,25)                                                     138500000
000172          WRITE(6,10)J, TIME                                              138600000
000203          WRITE(6,41)                                                     138700000
000207       41 FORMAT(/50X,29HZ-VELOCITY AT GRID POINT(M,N)/50X,29H----------- 138800000
             1--------------- )                                                 138900000
000207          WRITE(6,15) (N, N = 1, NZ)                                      139000000
000221          DO 50 M = 1, NW                                                 139100000
000224          DO 45 N = 1, NZ                                                 139200000
000225       45 CONVT(N) = VO*VZ(J,M,N)                                         139300000
000237       50 WRITE(6,21) M, (CONVT(N), N = 1, NZ)                            139400000
000260          WRITE(6,25)                                                     139500000
000264          WRITE(6,10)J, TIME                                              139600000
000275          WRITE(6,51)                                                     139700000
000301       51 FORMAT (/45X,40HGAS PHASE TEMPERATURE AT GRID POINT(M,N)/45X,   139800000
             140H---------------------------------------- )                     139900000
000301          WRITE(6,15) (N, N = 1, NZ)                                      140000000
000313          DO 60 M = 1, NW                                                 140100000
000316          DO 55 N = 1, NZ                                                 140200000
000317       55 CONVT(N) = TO*T(J,M,N)                                          140300000
000331       60 WRITE(6,21) M, (CONVT(N), N = 1, NZ)                            140400000
000352          WRITE(6,25)                                                     140500000
000356          WRITE(6,10)J, TIME                                              140600000
000367          WRITE(6,61)                                                     140700000
000373       61 FORMAT (/45X,46HTEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)/45X 140800000
             1,46H---------------------------------------------)                140900000
000373          WRITE(6,65) (N, N = 1, NZ)                                      141000000
000405       65 FORMAT(//2X,2HN=,2X,10(I6,6X)/2X,2HMS)                          141100000
000405          DO 70 MS = 1, NWS                                               141200000
000410          DO 68 N = 1, NZ                                                 141300000
000411       68 CONVT(N) = TSO*TS(J,MS,N)                                       141400000
000423       70 WRITE(6,21) MS, (CONVT(N), N = 1, NZ)                           141500000
000444          WRITE(6,75)                                                     141600000
000450       75 FORMAT(////20X,4HNOTE,10X,39HMS IS RADIAL GRID NUMBER IN SOLID PHA 141700000
             1SE/20X,4H----,10X,35HN IS GRID NUMBER IN AXIAL DIRECTION)         141800000
000450          DO 90 I = 1, NI                                                 141900000
000453          WRITE(6,10)J, TIME                                              142000000
000462          WRITE(6,78) I                                                   142100000
000470       78 FORMAT(/34X,26HMASS FRACTION OF SPECIES, ,I2,20H, AT GRID POINT(M, 142200000
             1N)/34X,48H------------------------------------------------ )      142300000
000470          WRITE(6,15) (N, N = 1, NZ)                                      142400000
```

```
000502          DO 90 M = 1, NW
000505       80 WRITE(6,21) M, (UYI(I,M,N), N = 1, NZ)
000532          WRITE(6,25)
000536       90 CONTINUE
000542          GO TO 900
          C-----
          C     PRINT OUT CALCULATED VALUES OF DEPENDENT VARIABLES.
          C-----
000543      829 NZ1 = NZ - 1
000545          NW1 = NW - 1
000547          NWS1 = NWS - 1
000550          WRITE(6,830) L,IT, TIME
000562      830 FORMAT (1H1,2X, 25HCALCULATED VALUES AT L = ,I4,7H, IT = ,I2,55X,
               17HTIME = ,G11.4,5H SEC./3X,20H-------------------- ,73X,4H---- )
000562          WRITE(6,831)
000566      831 FORMAT(/55X,26HDENSITY AT GRID POINT(M,N)/55X,26H-----------------
               1--------- )
000566          WRITE(6,15) (N, N = 1, NZ)
000600          DO 833 M = 1, NW
000603          DO 832 N = 1, NZ
000604      832 CONVT(N) = DENO*DEN(2,M,N)
000615      833 WRITE(6,834) M, (CONVT(N), N = 1, NZ)
000636      834 FORMAT(/2X,I2,2X,10G12.5 )
000636          WRITE(6,25)
000642          WRITE(6,830) L,IT,TIME
000654          WRITE (6,835)
000660      835 FORMAT(/55X,29HR-VELOCITY AT GRID POINT(M,N)/55X,29H-------------
               1--------------- )
000660          WRITE(6,15) (N, N = 1, NZ)
000672          M = 1
000673          DO 836 N = 1, NZ
000676      836 CONVT(N) = VO*VR(2,M,N)
000707          WRITE(6,834) M, (CONVT(N), N = 1, NZ)
000724          DO 838 M = 2, NW
000727          CONVT(1) = VO*VR(2,M,1)
000732          DO 837 N = 2, NZ
000734      837 CONVT(N) = VO*TEMPR(M,N)
000745      838 WRITE(6,834) M, (CONVT(N), N = 1, NZ)
000766          WRITE(6,25)
000772          WRITE(6,830) L,IT,TIME
001004          WRITE(6,839)
001010      839 FORMAT(/55X,29HZ-VELOCITY AT GRID POINT(M,N)/55X,29H-------------
               1--------------- )
```

```
001010          WRITE(6,15) (N, N = 1, NZ)                                      146800000
001022          M = 1                                                           146900000
001023          DO 840 N = 1, NZ                                                147000000
001026      840 CONVT(N) = VO*VZ(2,M,N)                                         147100000
001037          WRITE(6,834) M, (CONVT(N), N = 1, NZ)                           147200000
001054          DO 842 M = 2, NW1                                               147300000
001057          CONVT(1) = VO*VZ(2,M,1)                                         147400000
001062          DO 841 N = 2, NZ                                                147500000
001064      841 CONVT(N) = VO*TEMPZ(M,N)                                        147600000
001075      842 WRITE(6,834) M, (CONVT(N), N = 1, NZ)                           147700000
001116          M = NW                                                          147800000
001117          DO 843 N = 1, NZ                                                147900000
001121      843 CONVT(N) = VO*VZ(2,M,N)                                         148000000
001132          WRITE(6,834) M, (CONVT(N), N = 1, NZ)                           148100000
001147          WRITE(6,25)                                                     148200000
001153          WRITE(6,830) L,IT,TIME                                          148300000
001165          WRITE(6,844)                                                    148400000
001171      844 FORMAT (/50X,40HGAS PHASE TEMPERATURE AT GRID POINT(M,N)/50X,   148500000
           140H---------------------------------------- )                      148600000
001171          WRITE(6,15) (N, N = 1, NZ)                                      148700000
001203          DO 846 M = 1, NW                                                148800000
001206          CONVT(1) = TO*T(2,M,1)                                          148900000
001211          DO 845 N = 2, NZ                                                149000000
001213      845 CONVT(N) = TO*TEMPT(M,N)                                        149100000
001224      846 WRITE(6,834) M, (CONVT(N), N = 1, NZ)                           149200000
001245          WRITE(6,25)                                                     149300000
001251          WRITE(6,830) L,IT,TIME                                          149400000
001263          WRITE(6,848)                                                    149500000
001267      848 FORMAT (/45X,46HTEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)/45X  149600000
           1,46H---------------------------------------------)                  149700000
001267          WRITE(6,65) (N, N = 1, NZ)                                      149800000
001301          DO 850 MS = 1, NWS1                                             149900000
001304          CONVT(1) = TSO*TS(2,MS,1)                                       150000000
001307          DO 849 N = 2, NZ                                                150100000
001311      849 CONVT(N) = TSO*TEMPS(MS,N)                                      150200000
001321      850 WRITE(6,834) MS, (CONVT(N), N = 1, NZ)                          150300000
001342          MS = NWS                                                        150400000
001343          DO 851 N = 1, NZ                                                150500000
001345      851 CONVT(N) = TSO*TS(2,NWS,N)                                      150600000
001356          WRITE(6,834) MS, (CONVT(N), N = 1, NZ)                          150700000
001373          WRITE(6,75)                                                     150800000
001377          DO 857 I = 1, NI                                                150900000
001402          WRITE(6,830) L,IT,TIME                                          151000000
```

```
001413          WRITE (6,855) I
001421      855 FORMAT(/45X,26HMASS FRACTION OF SPECIES, ,I2,20H, AT GRID POINT(M,
               1N)/45X,48H------------------------------------------------ )
001421          WRITE(6,15) (N, N = 1, NZ)
001433          DO 856 M = 1, NWI
001436      856 WRITE (6,834) M, (YI(I,M,1), (TEMPY(I,M,N), N = 2, NZ)
001472          WRITE(6,834) NW, (UYI(I,NW,N), N = 1, NZ)
001514          WRITE(6,25)
001520      857 CONTINUE
001524      900 RETURN
001525          END
          C
```

```
              SUBROUTINE FORM2(J,UYI,UDI,UWI,UCPI,UHI)                  152300000
        C-----                                                          152400000
        C     THIS PROGRAM PRINTS ALL CALCULATED VALUES OF NON-DIMENSIONALIZED  152500000
        C     FUNCTIONS IN THEIR APPROPRIATE DIMENSIONS.                152600000
        C-----                                                          152700000
000011        DIMENSION UYI(3,20,10),UDI(3,20,10),UWI(3,20,10),UCPI(3,20,10),  152800000
             1UHI(3,20,10), CONVT(10)                                   152900000
        C-----                                                          153000000
000011        COMMON RO,AMUO,CO,WO,ALAMO,CPO,DENSO,ALAMSO,CSO,RRO,FC,   153100000
             1AMI(3),CAI(3),CPI(3),CCI(3),HSL(3),HIO(3),CP(2,20,10),HLG(3),  153200000
             2R(2,20,10), AMU(2,20,10), ALAM(2,20,10), HSGI(2,3,10),TBP(3),  153300000
             3DENS(2,15,10), CS(2,15,10), RR(2,10), ALAMS(2,15,10)      153400000
        C-----                                                          153500000
000011        COMMON/FORM/NW,NWS,NZ,NI,ANU1,ANU2,ANU3,CF,TC,TSC,FLL,FLU,L,IT,SF,  153600000
             1RA1,RA2,VO,TO,DENO,TSO,TIME,DEN(2,20,10),T(2,20,10),TS(2,15,10)  153700000
        C-----                                                          153800000
000011        DO 250 K = 1, 4                                           153900000
000012        WRITE(6,100) L, TIME                                      154000000
000021    100 FORMAT(1H1,2X,25HCALCULATED VALUES AT I = ,I4,65X,7HTIME = ,G11.4,  154100000
             1H SEC,/3X,20H-------------------- ,74X,4H---- )           154200000
000021        GO TO (110,120,130,140),K                                 154300000
000035    110 WRITE(6,115)                                              154400000
000041    115 FORMAT(/50X,27HPRESSURE AT GRID POINT(M,N)/50X,           154500000
             127H--------------------------- )                          154600000
000041        GO TO 150                                                 154700000
000045    120 WRITE(6,125)                                              154800000
000051    125 FORMAT(/50X,28HVISCOSITY AT GRID POINT(M,N)/50X,          154900000
             128H---------------------------- )                         155000000
000051        GO TO 150                                                 155100000
000055    130 WRITE(6,135)                                              155200000
000061    135 FORMAT(/45X,39HTHERMAL CONDUCTIVITY AT GRID POINT(M,N)/45X,  155300000
             139H---------------------------------------- )             155400000
000061        GO TO 150                                                 155500000
000065    140 WRITE(6,145)                                              155600000
000071    145 FORMAT (/45X,32HSPECIFIC HEAT AT GRID POINT(M,N)/45X,     155700000
             132H-------------------------------- )                     155800000
000071    150 WRITE(6,155) (N, N = 1, NZ)                               155900000
000103    155 FORMAT(//2X,2HN=,2X,10(I6,6X)/2X,2H M)                    156000000
000103        DO 210 M = 1, NW                                          156100000
000110        DO 200 N = 1, NZ                                          156200000
000111        GO TO (160,170,180,190), K                                156300000
000121    160 CONVT(N) = P(J,M,N)*DENO*VO*VO/(68000.)                   156400000
```

```
000132          GO TO 200                                                       156500000
000132      170 CONVT(N) = AMU(J,M,N)*AMUO                                      156600000
000141          GO TO 200                                                       156700000
000141      180 CONVT(N) = ALAM(J,M,N)*ALAMO                                    156800000
000150          GO TO 200                                                       156900000
000150      190 CONVT(N) = CP(J,M,N)*CPO                                        157000000
000157      200 CONTINUE                                                        157100000
000162      210 WRITE(6,230) M, (CONVT(N), N = 1, NZ)                           157200000
000204      230 FORMAT(/2X,I2,2X,10G12.5)                                       157300000
000204          WRITE(6,235)                                                    157400000
000210      235 FORMAT(////20X,4HNOTE,10X,36HM IS GRID NUMBER IN RADIAL DIRECTION/  157500000
               120X,4H----,10X,35HN IS GRID NUMBER IN AXIAL DIRECTION)          157600000
000210      250 CONTINUE                                                        157700000
000216          DO 380 I = 1, NI                                                157800000
000217          DO 380 K = 1, 4                                                 157900000
000220          WRITE(6,100) L, TIME                                            158000000
000227          GO TO (300,310,320,330), K                                      158100000
000243      300 WRITE(6,305) I                                                  158200000
000251      305 FORMAT (/35X,34HDIFFUSION COEFFICIENT OF SPECIES, ,I2,20H, AT GRID  158300000
               1 POINT(M,N)/35X,56H-------------------------------------------  158400000
               2--------- )                                                     158500000
000251          GO TO 340                                                       158600000
000255      310 WRITE(6,315) I                                                  158700000
000263      315 FORMAT (/35X,31HRATE OF PRODUCTION OF SPECIES, ,I2,20H, AT GRID PO  158800000
               1INT(M,N)/35X,53H---------------------------------------------  158900000
               2--- )                                                           159000000
000263          GO TO 340                                                       159100000
000267      320 WRITE(6,325) I                                                  159200000
000275      325 FORMAT (/32X,40HSPECIFIC HEAT PER UNIT MASS OF SPECIES, ,I2,20H, A  159300000
               1T GRID POINT(M,N)/32X,62H-------------------------------------  159400000
               2-------------------- )                                          159500000
000275          GO TO 340                                                       159600000
000301      330 WRITE(6,335) I                                                  159700000
000307      335 FORMAT(/35X,35HENTHALPY PER UNIT MASS OF SPECIES, ,I2,20H, AT GRID  159800000
               1 POINT(M,N)/35X,57H-------------------------------------------  159900000
               2---------- )                                                    160000000
000307      340 WRITE(6,155) (N, N = 1, NZ)                                     160100000
000321          DO 370 M = 1, NW                                                160200000
000326          DO 365 N = 1, NZ                                                160300000
000327          GO TO (345,350,355,360), K                                      160400000
000337      345 CONVT(N) = UDI(I,M,N)*DO                                        160500000
000346          GO TO 365                                                       160600000
000347      350 CONVT(N) = UWI(I,M,N)*WO                                        160700000
```

```
000356          GO TO 365                                                       160800000
000357      355 CONVT(N) = UCPI(I,M,N)*CPO                                      160900000
000366          GO TO 365                                                       161000000
000367      360 CONVT(N) = UHI(I,M,N)*CPO*TO                                    161100000
000377      365 CONTINUE                                                        161200000
000402      370 WRITE(6,230) M, (CONVT(N), N = 1, NZ)                           161300000
000424          WRITE(6,235)                                                    161400000
000430      380 CONTINUE                                                        161500000
000440          DO 455 K = 1, 3                                                 161600000
000442          WRITE(6,100) L, TIME                                            161700000
000451          GO TO (385,395,405), K                                          161800000
000464      385 WRITE(6,390)                                                    161900000
000470      390 FORMAT(/42X,41HDENSITY OF SOLID FUEL AT GRID POINT(MS,N)/42X,   162000000
             141H----------------------------------------- )                   162100000
000470          GO TO 415                                                       162200000
000474      395 WRITE(6,400)                                                    162300000
000500      400 FORMAT(/36X,54HTHERMAL CONDUCTIVITY OF SOLID FUEL AT GRID POINT(MS 162400000
             1,N)/36X,54H-------------------------------------------------------) 162500000
000500          GO TO 415                                                       162600000
000504      405 WRITE(6,410)                                                    162700000
000510      410 FORMAT(/34X,61HSPECIFIC HEAT PER UNIT MASS OF SOLID FUEL AT GRID P 162800000
             1OINT(MS,N)/34X,61H-------------------------------------------------- 162900000
             2------------- )                                                   163000000
000510      415 WRITE(6,420) (N, N= 1, NZ)                                      163100000
000522      420 FORMAT(//2X,2HN=,2X,10(I6,6X)/2X,2HMS)                          163200000
000522          DO 445 MS = 1, MWS                                              163300000
000527          DO 440 N = 1, NZ                                                163400000
000530          GO TO (425,430,435), K                                          163500000
000537      425 CONVT(N) = DENS(J,MS,N)*DENSO                                   163600000
000546          GO TO 440                                                       163700000
000546      430 CONVT(N) = ALAMS(J,MS,N)*ALAMSO                                 163800000
000555          GO TO 440                                                       163900000
000555      435 CONVT(N) = CS(J,MS,N)*CSO                                       164000000
000564      440 CONTINUE                                                        164100000
000567      445 WRITE(6,230) MS, (CONVT(N), N = 1, NZ)                          164200000
000611          WRITE(6,450)                                                    164300000
000615      450 FORMAT(////20X,4HNOTE,10X,39HMS IS RADIAL GRID NUMBER IN SOLID PHA 164400000
             1SE/20X,4H----,10X,35HN IS GRID NUMBER IN AXIAL DIRECTION)          164500000
000615      455 CONTINUE                                                        164600000
000623          WRITE(6,100) L, TIME                                            164700000
000632          WRITE(6,460)                                                    164800000
000636      460 FORMAT(/42X,43HREGRESSION RATE OF FUEL AT GRID POINT(MS,N)/42X,43H 164900000
             1------------------------------------------ )                      165000000
```

```
000636          WRITE(6,420) (N, N = 1, NZ)                                     165100000
000650          MS = 1                                                          165200000
000651          DO 465 N = 1, NZ                                                165300000
000656      465 CONVT(N) = RR(J,N)*RRO                                          165400000
000667          WRITE(6,230) MS, (CONVT(N), N = 1, NZ)                          165500000
000704          DO 480 I = 1, NT                                                165600000
000711          WRITE(6,470) I                                                  165700000
000715      470 FORMAT(//38X,32HHEAT OF SUBLIMATION OF SPECIES, ,I2,20H, AT GRID P   165800000
               1OINT(M,N)/38X,54H-----------------------------------------------------   165900000
               2-----//)                                                        166000000
000716          DO 475 N = 1, NZ                                                166100000
000723      475 CONVT(N) = HSGI(J,I,N)*CSO*TSO                                  166200000
000737          WRITE(6,230) MS, (CONVT(N), N = 1, NZ)                          166300000
000753      480 CONTINUE                                                        166400000
000761          WRITE(6,450)                                                    166500000
000765          RETURN                                                          166600000
000766          END                                                             166700000
          C                                                                     166800000
```

```
                FUNCTION UCT(J,K,U)
          C-----
          C     THIS FUNCTION CALCULATES THE VALUE OF A VARIABLE AT L+1/2
          C     M-1/2 AND N-1/2.
          C     TWO IS THE MINIMUM VALUE TO BE ASSIGNED TO EITHER J OR K.
          C-----
000006          DIMENSION U(2,20,10)
          C-----
000006          JA = J-1
000010          KA = K-1
000011          UCT = (U(2,J,K)+U(2,J,KA)+U(2,JA,K)+U(2,JA,KA)+U(1,J,K)+U(1,J,KA)+
               1U(1,JA,K)+U(1,JA,KA))/8.0
000045          RETURN
000045          END
          C
```

```
              FUNCTION UCTI(II,J,K,UI1,UI2)                                     168400000
        C-----                                                                  168500000
        C     THIS FUNCTION CALCULATES THE VALUE OF A I-SUBSCRIPTED VARIABLE    168600000
        C     AT L+1/2, M-1/2 AND N-1/2.                                        168700000
        C     TWO IS THE MINIMUM VALUE TO BE ASSIGNED TO EITHER J OR K.         168800000
        C-----                                                                  168900000
000010        DIMENSION UI1(3,20,10), UI2(3,20,10)                              169000000
        C-----                                                                  169100000
000010        JA = J-1                                                          169200000
000012        KA = K-1                                                          169300000
000013        UCTI = (UI2(II,J,K)+UI2(II,J,KA)+UI2(II,JA,K)+UI2(II,JA,KA)+      169400000
             1UI1(II,J,K)+UI1(II,J,KA)+UI1(II,JA,K)+UI1(II,JA,KA))/8.0          169500000
000057        RETURN                                                            169600000
000057        END                                                               169700000
        C                                                                       169800000
```

```
                FUNCTION URCT(J,K,U)
          C-----
          C     THIS FUNCTION CALCULATES THE R-DERIVATIVE OF ANY VARIABLE AT
          C     L+1/2, M-1/2 AND N-1/2.
          C     TWO IS THE MINIMUM VALUE TO BE ASSIGNED TO EITHER J OR K.
          C-----
000006          DIMENSION U(2,20,10)
          C-----
000006          COMMON/FUN/DELR,DELZ,R(20)
          C-----
000006          JA = J-1
000010          KA = K-1
000011          URCT = ((U(2,J,K)-U(2,JA,K))+(U(2,J,KA)-U(2,JA,KA))+(U(1,J,K)-
               1U(1,JA,K))+(U(1,J,KA)-U(1,JA,KA)))/(4.0*DELR)
000047          RETURN
000047          END
          C
```

```
                FUNCTION UZCT(J,K,U)
          C-----
          C     THIS FUNCTION CALCULATES THE Z-DERIVATIVE OF ANY VARIABLE AT
          C     L+1/2, M-1/2 AND N-1/2.
          C     TWO IS THE MINIMUM VALUE TO BE ASSIGNED TO EITHER J OR K.
          C-----
000006          DIMENSION U(2,20,10)
          C-----
000006          COMMON/FUN/DELR,DELZ,R(20)
          C-----
000006          JA = J-1
000010          KA = K-1
000011          UZCT = ((U(2,J,K)-U(2,J,KA))+(U(2,JA,K)-U(2,JA,KA))+(U(1,J,K)-
               1U(1,J,KA))+(U(1,JA,K)-U(1,JA,KA)))/(4.0*DELZ)
000046          RETURN
000046          END
```

APPENDIX C

PROGRAM PLOT

This computer program utilizes the punched card output from computer program HETCOMB to display the computed results through the use of Calcomp plotter as shown in the figures of Chapter VII. Axial profiles of density, radial velocity, axial velocity, temperature in gas phase, mass fraction of oxygen, mass fraction of aluminum, mass fraction of aluminum oxide and temperature in solid phase are plotted. Three types of data can be used for plottting. They are: (a) initial profiles, (b) profiles at any instant of time, and, (c) profiles at any axial position.

The first two input cards determines the type of data to be plotted. The first input card consists of seven numbers punched according to the format (7F8.0). They are identified by the following symbols: DELZ, DELRS, TO VO, DENO, TSO and TIMEI. The first six symbols have the same meaning as that in computer program HETCOMB. TIMEI is defined either as the actual time in seconds or the time increment in seconds between successive curves in a plot.

The second input card consists of 15 numbers punched according to the format (15I4). They are called by the following symbols: NW, NWS, NR, NRS, NX, NXS, NZI, NZ, ND, NP, NMAX, NMAXS, NSET, J and I. The first six symbols have the same meaning as that in computer program HETCOMB. The remaining symbols are defined as follows:

NZI = First axial grid number;

NZ = Last axial grid number;

ND = Difference between successive axial grid number to be plotted;

NP = Number of curves in each plot;

NMAX = Number of radial grid points in the gas phase to be plotted;

NMAXS = Number of radial grid points in the solid phase to be plotted;

NSET = Number of sets to be plotted;

J = 1 for plotting profiles at any instant of time; any number other than 1 for plotting profiles at any axial position;

I = 0 for plotting data only; any number other than 0 for plotting data and fitted curves.

The curve fitting subroutine employs a third-degree natural spline function to interpolate the given data points based on a modified version of a program listing reported by Greville.[1]

A listing of computer program PLOT is shown as follows:

[1]Greville, T. N. E., "Spline Functions, Interpolation, and Numerical Quadrature," Mathematical Methods for Digital Computers, Vol. II, eds. Anthony Ralston and Herbert S. Wilf (New York, John Wiley and Sons, 1967), pp. 156-68.

Listing of Program Plot

```
                PROGRAM PLOT (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
000003          DIMENSION TIME(5), Z(5), YY(5)
000003          COMMON X(30),Y(30),XINT( 80),VARD(30,5),FUNC(5, 30),FUNC1(5, 80),
               1FUNC2(5, 80),AB(30,5),AC(30,5),AD(30,5),AA(5),YINT( 80)
000003          CALL CALCOMP
000004          READ(5,5) DELZ,DELKS,TO,VO,CENO,TSO,TIME1
000026        5 FORMAT(7F8.0)
000026          READ(5,10) NW,NWS,NR,NRS,NX,NXS,NZ1,NZ,ND,NP,NMAX,NMAXS,NSET,J,I
000070       10 FORMAT(15I4)
000070          MR1 = NW+1-NR
000073          MR2 = NR-2
000074          DELX = 1.0/(NX*MR2+MR1)
000102          XPG = 5.0
000103          XDV = 20.0
000105          XTIC = 0.5
000106          YPG = 5.0
000107          YDV = 20.0
000110          YTIC = 0.5
000111          NMA = NMAX + 1
000113          NMB = NMAX + 2
000114          NMC = NMAX + 3
000116          NSA = NMAXS + 1
000117          NSB = NMAXS + 2
000120          NSC = NMAXS + 3
000121          DO 12 L = 1, NP
000122       12 TIME(L) = (L-1)*TIME1
000131          NN = 0
000132          DO 14 N = NZ1, NZ, ND
000134          NN = NN + 1
000136       14 Z(NN)= (N-1)*DELZ
000144          DO 999 NL = 1, NSET
000146          DO 40 M = 1, NMAX
000147          M1 = M -1
000151          IF(M1-MR1)20, 20, 30
000153       20 X(M) = M1*DELX
000156          GO TO 40
000157       30 X(M) = (MR1+NX*(M1-MR1))*DELX
000166       40 CONTINUE
000171          DO 800 NN = 1, 7
000172          DO 210 LL= 1, NP
000173          MA = NW
000175          MB = NW-1
```

```
000175          MC = Nw-2
000200          MD = Nw-3
000201          ME = Nw-4
000203          MM = Nw/5
000205          DO 200 M = 1, MM
000207          READ(5,100) Y(MA),Y(MB),Y(MC),Y(MD),Y(ME)
000224      100 FORMAT(5G12.5)
000224          MA = MA - 5
000225          MB = MB - 5
000227          MC = MC - 5
000230          MD = MD - 5
000231          ME = ME - 5
000232      200 CONTINUE
000234          IF(NN-2) 206, 202, 206
000236      202 DO 204 M = 1, Nw
000240      204 Y(M) = -Y(M)
000244      206 DO 210 M = 1, Nw
000246          VARD(M,LL) = Y(M)
000253      210 CONTINUE
000260          GO TO (240,230,240,220,240,240,230), NN
000273      220 Y(NMA) = 0.5
000275          GO TO 245
000275      230 Y(NMA) = 0.07
000300          GO TO 245
000301      240 Y(NMA) = 0.0
000303      245 CALL ASCALE(X,XPG,NMAX,1,XDV)
000307          CALL ASCALE(Y,YPG,NMA,1,YDV)
000313          Y(NMA) = Y(NMB)
000316          Y(NMB) = Y(NMC)
000320          CALL AXES(0.,0.,0.,XPG,X(NMA),X(NMB),XTIC,XDV,32HDIMENSIONLESS DIS
               ITANCE FROM WALL..14,-32)
000332      250 GO TO (310,320,330,340,350,360,370), NN
000345      310 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,21HDIMENSIONLESS DE
               INSITY..14,21)
000361          DO 315 LL = 1, NP
000363          DO 312 M = 1, NMAX
000364      312 Y(M) = VARD(M,LL)
000374      315 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
000406          CALL NOTATE(2.46,2.0,.14,39,0.0,-1)
000412          CALL NOTATE(2.6,1.97,.09,1HC,0.0,1)
000416          CALL NUMBER(3.06,2.0,.14,DEN0,0.,3)
000422          CALL NOTATE(2.84,2.0,.14,18H=       LBM./CU.FT.,0.0,18)
000426          CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
```

```
000436          GO TO 400
000437      320 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,29HDIMENSICNLESS RA
               1DIAL VELOCITY,.14,29)
000453          DO 325 LL = 1, NP
000455          DO 322 M = 1, NMAX
000456      322 Y(M) = VARD(M,LL)
000466      325 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
000500          CALL NOTATE(2.84,3.5,.14,18HV  =       FT./SEC.,0.0,18)
000504          CALL NOTATE(2.95,3.47,.09,1H0,0.0,1)
000510          CALL NUMBER(3.44,3.5,.14,VC,0.0,1)
000514          CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
000524          GO TO 400
000525      330 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,28HDIMENSICNLESS AX
               1IAL VELOCITY,.14,28)
000541          DO 335 LL = 1, NP
000543          DO 332 M = 1, NMAX
000544      332 Y(M) = VARD(M,LL)
000554      335 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
000566          CALL NOTATE(2.84,1.5,.14,18HV  =       FT./SEC.,0.0,18)
000572          CALL NOTATE(2.95,1.47,.09,1H0,0.0,1)
000576          CALL NUMBER(3.44,1.5,.14,VC,0.0,1)
000602          CALL INTRE(I,NP,NMAX, 50,.0040,0.0,1,1)
000612          GO TO 400
000613      340 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,25HDIMENSIONLESS TE
               1MPERATURE,.14,25)
000627          DO 345 LL = 1, NP
000631          DO 342 M = 1, NMAX
000632      342 Y(M) = VARD(M,LL)
000642      345 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
000654           CALL NOTATE(3.20,3.5,.14,15HT  =          R.,0.0,15)
000660          CALL NOTATE(3.32,3.47,.09,1H0,0.0,1)
000664           CALL NUMBER(3.88,3.5,.14,TC,0.0,1)
000670          CALL NOTATE(4.64,3.58,.09,1H0,0.0,1)
000674          CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
000704          GO TO 400
000705      350 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,23HMASS FRACTION OF
               1 OXYGEN,.14,23)
000721          DO 355 LL = 1, NP
000723          DO 352 M = 1, NMAX
000724      352 Y(M) = VARD(M,LL)
000734      355 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
000746          CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
000755          GO TO 400
```

```
000756     360 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,25HMASS FRACTION OF
               1 ALUMINUM,.14,25)
000772         DO 365 LL = 1, NP
000774         DO 362 M = 1, NMAX
000775     362 Y(M) = VARD(M,LL)
001005     365 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
001017         CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
001026         GO TO 400
001027     370 CALL AXES(0.,0.,90.,YPG,Y(NMA),Y(NMB),YTIC,YDV,31HMASS FRACTION OF
               1 ALUMINUM OXIDE,.14,31)
001043         DO 385 LL = 1, NP
001045         DO 382 M = 1, NMAX
001046     382 Y(M) = VARD(M,LL)
001056     385 CALL LINPLT(X,Y,NMAX,1,-1,LL,1,0)
001070         CALL INTRE(I,NP,NMAX, 50,.0040,0.0,0,1)
001077     400 CALL NOTATE(1.50,7.9,.14,17HFIGURE (         ),0.,17)
001103         DO 610 L = 1, NP
001105         YY(L) = 6.6-.25*(L-1)
001112     610 CALL PNTPLT(3.2,YY(L)+.06,L,1)
001122         IF(TIME1-0.0) 700, 650, 700
001124     650 CALL NOTATE(0.82,7.6,.14,28HINITIAL PROFILE IN GAS PHASE,0.,28)
001130         DO 680 L = 1, NP
001132         CALL NOTATE(3.56,YY(L)+.14,.14,23,0.0,-1)
001140         IF(L-1) 670, 660, 670
001142     660 CALL NOTATE(3.56,YY(L),.14,7HZ = 0.0,0.0,7)
001147         GO TO 680
001150     670 CALL NOTATE(3.56,YY(L),.14,7HZ > 0.0,0.0,7)
001155     680 CONTINUE
001160         GO TO 800
001160     700 CALL NOTATE(1.76,7.3,.14,12HIN GAS PHASE,0.,12)
001164         IF(J-1) 750, 730, 750
001166     730 CALL NOTATE(0.82,7.6,.14,29HPROFILE AT TIME =        SEC.,0.,29)
001172         CALL NUMBER(2.90,7.6,.14,TIME1,0.,5)
001176         DO 740 L = 1, NP
001200         CALL NOTATE(3.56,YY(L)+.14,.14,23,0.0,1)
001206         CALL NOTATE(3.56,YY(L),.14,3HZ =,0.0,3)
001213     740 CALL NUMBER(4.04,YY(L),.14,Z(L),0.,2)
001223         GO TO 800
001223     750 CALL NOTATE(.46,7.6,.14,35HPROFILE AT AXIAL POSITION, Z =    ,,0.,
               135)
001227         CALL NOTATE(3.70,7.74,.14,23,0.0,-1)
001233         CALL NUMBER(4.08,7.6,.14,Z(NL),0.,2)
001240         DO 760 L = 1, NP
```

```
001242          CALL NUMBER(3.56,YY(L),.14,TIME(L),0.,4)
001246      780 CALL NOTATE(4.40,YY(L),.14,4HSEC.,0.,4)
001256      800 CALL CALPLT(12.,0.,-3)
001263          DO 840 MS = 1, NMAXS
001265          IF(MS-NRS) 820,830,830
001267      820 X(MS) = (MS-1)*DELRS + 1.0
001275          GO TO 840
001275      830 X(MS) = 1.0 + (NXS*(MS+1-NRS)+NRS-2)*DELRS
001307      840 CONTINUE
001312          DO 860 LL= 1, NP
001313          READ(5,850) (Y(N), N = 1, NKS)
001325      850 FORMAT(5G12.5)
001325          DO 860 M = 1, NMAXS
001327          VARD(M,LL) = Y(M)
001334      860 CONTINUE
001341          Y(NSA) = 0.0
001342          CALL ASCALE(X,XPG,NMAXS,1,XDV)
001346          CALL ASCALE(Y,YPG,NSA,1,YDV)
001352          Y(NSA) = Y(NSB)
001355          Y(NSB) = Y(NSC)
001357          CALL AXES(0.,0.,0.,XPG,X(NSA  ),X(NSB  ),XTIC,XDV,29HDIMENSIONLESS
               1 RADIAL DISTANCE,.14,-29)
001371          CALL AXES(0.,0.,90.,YPG,Y(NSA),Y(NSB),YTIC,YDV,25HDIMENSICNLESS TE
               1MPERATURE,.14,25)
001405          DO 865 LL = 1, NP
001407          DO 862 M = 1, NMAXS
001410      862 Y(M) = VARD(M,LL)
001420      865 CALL LINPLT(X,Y,NMAXS,1,-1,LL,1,0)
001432          CALL NOTATE(3.20,3.5,.14,15HTS  =        R.,0.0,15)
001436          CALL NOTATE(3.44,3.47,.09,1H0,0.0,1)
001442          CALL NUMBER(4.00,3.5,.14,TSC,C.0,1)
001446          CALL NOTATE(4.64,3.53,.09,1H0,0.0,1)
001452          CALL INTRF(1,NP,NMAXS, 50,.0003,1.0,0,1)
001462          CALL NOTATE(1.50,7.9,.14,17HFIGURE (        ),0.,17)
001466          DO 902 L = 1, NP
001470      902 CALL PNTPLT(3.2,YY(L)+.06,L,1)
001500          IF(TIME1-0.0) 910, 905, 910
001502      905 CALL NOTATE(0.72,7.6,.14,30HINITIAL PROFILE IN SOLID PHASE,0.,30)
001506          DO 908 L = 1, NP
001510          CALL NOTATE(3.56,YY(L)+.14,.14,23,0.0,-1)
001514          IF(L-1) 907, 906, 907
001520      906 CALL NOTATE(3.56,YY(L),.14,7HZ = 0.0,0.0,7)
001525          GO TO 908
```

```
001526      907 CALL NOTATE(3.55,YY(L),.14,7HZ > 0.0,0.0,7)
001533      908 CONTINUE
001536          GO TO 999
001536      910 CALL NOTATE(1.66,7.3,.14,14HIN SOLID PHASE,0.,14)
001542          IF(J-1) 920, 915, 920
001544      915 CALL NOTATE(0.82,7.6,.14,29HPROFILE AT TIME =        SEC.,0.,29)
001550          CALL NUMBER(2.90,7.6,.14,TIME1,0.,5)
001554          DO 918 L = 1, NP
001556          CALL NOTATE(3.56,YY(L)+.14,.14,23,0.0,-1)
001564          CALL NOTATE(3.55,YY(L),.14,3HZ =,0.0,3)
001571      918 CALL NUMBER(4.04,YY(L),.14,Z(L),0.,2)
001601          GO TO 999
001601      920 CALL NOTATE(.46,7.6,.14,35HPROFILE AT AXIAL POSITION, Z =    ,0.,
               135)
001605          CALL NOTATE(3.70,7.74,.14,23,0.0,-1)
001611          CALL NUMBER(4.08,7.6,.14,Z(NL),0.,2)
001616          DO 930 L = 1, NP
001620          CALL NUMBER(3.56,YY(L),.14,TIME(L),0.,4)
001624      930 CALL NOTATE(4.40,YY(L),.14,4HSEC.,0.,4)
001634      999 CALL CALPLT(12.,0.,-3)
001642          CALL CALPLT(0.0,999)
001644          STOP
001646          END
```

```
              SUBROUTINE INTRE(II,NP,NMAX,K,DEL,XO,NVV,NPP)
000013        COMMON X(30),Y(30),XINT( 80),VARD(30,5),FUNC(5, 80),FUNC1(5, 80),
             1FUNC2(5, 80),AB(30,5),AC(30,5),AD(30,5),AA(5),YINT( 80)
000013        IF(II-0) 100, 999, 100
000014    100 DO 200 M = 1, K
000016    200 XINT(M) = (M-1)*DEL+XO
000025        J = 0
000026        CALL SPLINE(30,5, 80,NMAX,NP,K,X,VARD,XINT,.0000000001,AA,FUNC,
             1FUNC1,FUNC2,AB,AC,AD,Y,J,1)
000053        IF(X(NMAX)-XINT(K)) 220, 220, 240
000064    220 STOP3
000066    240 DO 300 M = 1, NMAX
000070        IF(X(M)-XINT(K)) 300, 300, 400
000075    300 CONTINUE
000100    400 KK = K
000101        DO 600 MM = 4, NMAX
000103        KK=KK + 1
000105        XINT(KK)= X(MM)
000110        DO 500 L = 1, NP
000112    500 FUNC(L,KK) = VARD(MM,L)
000125    600 CONTINUE
000130        XINT(KK+1) = X(NMAX+1)
000132        XINT(KK+2) = X(NMAX+2)
000134        KMAX = KK
000136        IF(NVV-1) 630, 610, 630
000140    610 DO 620 L = 1, NPP
000142        DO 620 M = 1, KMAX
000143    620 FUNC(L,M) = XINT(M)**(1.0/7.0)
000165    630 WRITE(6,650) KMAX
000173    650 FORMAT(/10X,I3)
000173        WRITE(6,700) ((XINT(N),FUNC(L,N), N = 1, KMAX), L = 1, NP)
000232    700 FORMAT(/2X,2G12.5,6X,2G12.5,6X,2G12.5,2X,2G12.5)
000232        YINT(KMAX+1) = Y(NMAX+1)
000241        YINT(KMAX+2) = Y(NMAX+2)
000243        DO 900 L = 1, NP
000244        DO 880 M = 1, KMAX
000245    880 YINT(M) = FUNC(L,M)
000256        CALL LINPLT(XINT,YINT,KMAX,1,0,0,0,0)
000266    900 CONTINUE
000274    999 RETURN
000275        END
```

```
              SUBROUTINESPLINE(MNPTS,MNCVS,MMAX,N,NCVS,M,X,Y,T,EPS,PROXIN,SS,SS1
             1,SS2,S2,S3,DELY,H,IW,ITG)
000027        DIMENSION X(MNPTS),Y(MNPTS,MNCVS),T(MMAX),DELY(MNPTS,MNCVS),
             1S2(MNPTS,MNCVS),S3(MNPTS,MNCVS),SS1(MNCVS,MMAX),SS(MNCVS,MMAX) ,
             A H(MNPTS)       ,SS2(MNCVS,MMAX),PROXIN(MNCVS),
             2       B(50),DELSQY(50),H2(50),C(50)
000027        EPSLN=EPS
000030        IF(IW)15,2,15
000032      2 N1=N-1
000034        IW=2
000035        DO 101 K=1,NCVS
000037      3 DO 51 I=1,N1
000041        H(I)=X(I+1)-X(I)
000046        II=I+1
000047     51 DELY(I,K)=(Y(II,K)-Y(I,K))/ H(I)
000066      4 DO 52 I=2,N1
000070        II=I-1
000072        H2(I)=H(II)   +H(I)
000077        DELSQY(I)=(DELY(I,K)-DELY(II,K))/ H2(I)
000113        B(I)=.5*H(II)  /H2(I)
000120        S2(I,K)=2.*DELSQY(I)
000125     52 C(I)=3.* DELSQY(I)
000132        S2(1,K)=0.0
000134        S2(N,K)=0.0
000136        OMEGA=1.0717968
000137      5 ETA=0.
000140      6 DO 10 I=2,N1
000142        IB=I-1
000144        IF=I+1
000145      7 W=(C(I)-B(I)*S2(IB,K)-(.5-B(I))*S2(IF,K)-S2(I,K))*OMEGA
000172      8 IF (ABS(W)-ETA) 10,10,9
000176      9 ETA=ABS(W)
000200     10 S2(I,K)=S2(I,K)+W
000210     13 IF (ETA-EPSLN) 14,5,5
000213     14 DO 53 I=1,N1
000215        II=I+1
000217     53 S3(I,K)=(S2(II,K)-S2(I,K))/ H(I)
000237    101 CONTINUE
000242     15 CONTINUE
000242    104 J=0
000243    105 J=J+1
000245     16 I=1
```

```
000246      54 IF (T(J)-X(1)) 58,17,55
000253      55 IF (T(J)-X(N)) 57,59,58
000261      56 IF (T(J)-X(I)) 60,17,57
000267      57 I=I+1
000271         GO TO 56
000271      58 PRINT 44, J
000277      44 FORMAT (I4,24HTH ARGUMENT OUT OF RANGE)
000277         GO TO 61
000303      59 I=N
000304      60 I=I-1
000306      17 DO 110 K=1,NCVS
000310         HT1=T(J)-X(I)
000316         II=I+1
000317         HT2=T(J)-X(II)
000324         PROD=HT1 * HT2
000325         SS2(K,J)=S2(I,K)+HT1*S3(I,K)
000342         DELSQS=(S2(I,K)+S2(II,K)+SS2(K,J))/6.
000357         SS(K,J)=Y(I,K)+HT1*DELY(I,K)+FRCO*DELSQS
000374         SS1(K,J)=DELY(I,K)+(HT1+HT2)*DELSQS+PROD*S3(I,K)/6.0
000414     110 CONTINUE
000416      61 CONTINUE
000416         IF(J.LT.M)GO TO 105
000420         IF(ITG.GT.0)RETURN
000423         DO 120 K=1,NCVS
000425      20 PROXIN(K)=0.0
000430         DO 62 I=1,N1
000431         II=I+1
000433      62 PROXIN(K)=PROXIN(K)+.5*H(I)  *(Y(I,K)+Y(II,K))-H(I)  **3*(
           1S2(I,K)+S2(II,K))/24.
000467     120 CONTINUE
000471         RETURN
000472         END
```

APPENDIX D

TABULATED RESULTS OF ALL THE DEPENDENT VARIABLES

With 2.0 and 1.0 as the modified values for the reaction orders of aluminum and oxygen respectively, numerical calculations for the simple case as described in Chapter VI have been performed. The computer results for all the dependent variables at $t \approx 0.003$, 0.006 and 0.009 seconds are tabulated as shown in the following tables. Selected data are plotted in figures in Chapter VII.

Table D-1.1 - D-1.8 Computed Results for All the Dependent Variables at $t \simeq 0.003$ Sec with Modified Values for the Reaction Orders

Table D-1.1

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

DENSITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.13500	.13359	.13238	.13108	.12982	.12863	.12764	.12700	.12672	.12664
2	.13500	.13359	.13238	.13108	.12982	.12863	.12764	.12700	.12672	.12664
3	.13500	.13447	.13394	.13340	.13288	.13240	.13201	.13178	.13164	.13147
4	.13500	.13333	.13267	.13151	.13037	.12931	.12843	.12788	.12768	.12762
5	.13500	.13451	.13402	.13355	.13310	.13271	.13244	.13232	.13225	.13207
6	.13500	.13335	.13269	.13154	.13040	.12933	.12847	.12797	.12782	.12781
7	.13500	.13449	.13400	.13353	.13311	.13276	.13257	.13256	.13257	.13241
8	.13500	.13333	.13265	.13147	.13030	.12922	.12838	.12794	.12786	.12788
9	.13500	.13445	.13392	.13342	.13299	.13269	.13260	.13272	.13290	.13267
10	.13500	.13354	.13228	.13092	.12960	.12843	.12756	.12715	.12710	.12709
11	.13500	.13441	.13385	.13332	.13286	.13256	.13252	.13270	.13279	.13261
12	.13500	.13353	.13223	.13084	.12949	.12829	.12742	.12703	.12699	.12702
13	.13500	.13438	.13380	.13325	.13277	.13245	.13237	.13251	.13264	.13261
14	.13500	.13353	.13216	.13069	.12913	.12748	.12587	.12473	.12445	.12482
15	.13500	.13433	.13367	.13285	.13145	.12885	.12511	.12184	.12101	.12241
16	.13500	.13354	.13148	.12943	.12463	.11600	.10529	9.76849E-02	9.63997E-02	9.91762E-02
17	.13500	.13370	.13296	.12934	.11938	.10257	8.72173E-02	8.05424E-02	8.02977E-02	8.11020E-02
18	.13500	.13323	.13014	.12108	.10075	8.22402E-02	8.18938E-02	.10264	8.77689E-02	6.95814E-02
19	.13500	.13273	.12716	.10989	7.19845E-02	8.24435E-02	6.88021E-02	7.64066E-02	8.29053E-02	7.57546E-02
20	.13500	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382

Table D-1.2

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

GAS PHASE TEMPERATURE AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	3240.0	3271.9	3304.1	3336.8	3369.3	3400.4	3426.8	3443.6	3446.7	3427.9
2	3240.0	3271.9	3304.1	3336.8	3369.3	3400.4	3426.8	3443.6	3446.7	3427.9
3	3240.0	3252.8	3265.8	3278.8	3291.7	3303.7	3313.4	3318.7	3317.8	3301.1
4	3240.0	3268.2	3296.9	3326.0	3355.0	3382.6	3405.7	3419.7	3420.9	3401.4
5	3240.0	3251.8	3263.6	3275.1	3286.2	3295.9	3302.6	3305.0	3302.5	3285.9
6	3240.0	3267.3	3296.3	3325.3	3354.4	3381.9	3404.5	3417.4	3417.1	3396.5
7	3240.0	3252.2	3264.1	3275.6	3286.1	3294.6	3299.3	3299.0	3294.6	3277.5
8	3240.0	3268.2	3297.3	3327.1	3356.9	3384.9	3406.9	3418.1	3416.1	3394.6
9	3240.0	3253.3	3266.1	3278.3	3288.9	3296.4	3298.5	3295.1	3288.8	3271.0
10	3240.0	3273.0	3306.7	3341.0	3374.9	3405.9	3429.0	3439.4	3436.5	3415.9
11	3240.0	3254.1	3267.8	3280.9	3292.2	3299.6	3300.5	3295.5	3289.0	3272.6
12	3240.0	3273.3	3307.8	3343.0	3377.8	3409.4	3432.6	3442.7	3439.5	3417.9
13	3240.0	3254.3	3269.2	3282.6	3294.4	3302.4	3304.3	3300.1	3292.8	3272.7
14	3240.0	3274.0	3309.5	3346.9	3387.2	3430.9	3474.4	3505.1	3508.8	3477.6
15	3240.0	3256.2	3272.3	3292.3	3326.8	3392.4	3491.3	3582.4	3602.3	3541.2
16	3240.0	3275.5	3315.5	3378.6	3505.8	3760.5	4134.1	4449.5	4503.2	4356.2
17	3240.0	3259.2	3289.1	3378.9	3656.9	4259.5	5055.3	5554.4	5543.2	5356.4
18	3240.0	3280.7	3355.8	3604.4	4378.1	5641.6	6840.0	6840.0	6840.0	6840.0
19	3240.0	3267.3	3354.2	3898.7	6825.1	6840.0	6840.0	6840.0	6840.0	6840.0
20	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0

Table D-1.3

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

Z-VELOCITY AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000
2	19.746	19.775	19.806	19.838	19.870	19.902	19.929	19.947	19.951	19.945
3	19.470	19.477	19.484	19.489	19.493	19.495	19.495	19.494	19.494	19.495
4	19.169	19.200	19.232	19.266	19.301	19.335	19.365	19.384	19.387	19.378
5	18.835	18.844	18.851	18.857	18.861	18.862	18.860	18.856	18.855	18.857
6	18.463	18.495	18.528	18.563	18.599	18.635	18.666	18.685	18.685	18.674
7	18.040	18.049	18.057	18.063	18.067	18.067	18.062	18.056	18.053	18.057
8	17.546	17.578	17.612	17.647	17.685	17.722	17.754	17.771	17.768	17.755
9	16.952	16.966	16.979	16.990	16.998	16.999	16.992	16.982	16.981	16.987
10	16.723	16.775	16.826	16.877	16.928	16.978	17.018	17.036	17.025	17.005
11	16.473	16.466	16.460	16.455	16.446	16.431	16.410	16.394	16.400	16.416
12	16.138	16.246	16.294	16.342	16.392	16.445	16.491	16.509	16.489	16.458
13	15.932	15.889	15.894	15.878	15.865	15.837	15.801	15.780	15.794	15.817
14	15.546	15.539	15.631	15.678	15.731	15.795	15.853	15.872	15.839	15.805
15	15.146	15.147	15.144	15.136	15.114	15.068	15.010	14.986	15.025	15.074
16	14.671	14.701	14.735	14.774	14.825	14.897	14.969	14.984	14.928	14.889
17	14.080	14.073	14.062	14.025	13.943	13.793	13.616	13.550	13.645	13.727
18	13.298	13.243	13.133	12.961	12.706	12.406	12.224	12.227	12.154	12.000
19	12.035	11.142	10.298	9.3615	8.1367	6.9115	6.4135	6.7481	7.0702	6.8338
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-I.4

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

R-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	-1.05957E-03	-2.16090E-03	-3.27780E-03	-4.23353E-03	-4.82582E-03	-4.30412E-03	-2.34373E-03	2.54213E-04	1.52437E-03
3	0.	1.31532E-03	2.69118E-03	4.10247E-03	5.38405E-03	6.07606E-03	5.40145E-03	2.90088E-03	-3.49330E-04	-1.86778E-03
4	0.	-1.90820E-03	-3.90946E-03	-5.97323E-03	-7.85500E-03	-8.86313E-03	-7.82784E-03	-4.08715E-03	6.71574E-04	2.74354E-03
5	0.	2.26106E-03	4.55043E-03	7.14305E-03	9.44358E-03	1.06886E-02	9.40179E-03	4.77500E-03	-9.90828E-04	-3.29677E-03
6	0.	-2.80951E-03	-5.78770E-03	-8.91263E-03	-1.18129E-02	-1.33694E-02	-1.16593E-02	-5.68973E-03	1.53883E-03	4.11921E-03
7	0.	3.26700E-03	6.62756E-03	1.02534E-02	1.36559E-02	1.54816E-02	1.33859E-02	6.24257E-03	-2.11708E-03	-4.66909E-03
8	0.	-3.71432E-03	-7.69166E-03	-1.19412E-02	-1.59646E-02	-1.81115E-02	-1.55063E-02	-6.88605E-03	2.82560E-03	5.22884E-03
9	0.	4.23041E-03	8.74378E-03	1.35860E-02	1.81886E-02	2.05376E-02	1.71298E-02	6.67914E-03	-4.38307E-03	-6.20969E-03
10	0.	-6.50635E-03	-1.27586E-02	-1.90885E-02	-2.49372E-02	-2.77134E-02	-2.27166E-02	-8.60285E-03	5.18588E-03	5.97251E-03
11	0.	9.23515E-03	1.74165E-02	2.51564E-02	3.19297E-02	3.42255E-02	2.57875E-02	5.68538E-03	-1.21133E-02	-1.15258E-02
12	0.	-1.24795E-02	-2.30517E-02	-3.29375E-02	-4.16102E-02	-4.51402E-02	-3.54256E-02	-1.14975E-02	8.64416E-03	6.22326E-03
13	0.	1.54023E-02	2.80763E-02	3.96336E-02	4.94969E-02	5.12256E-02	3.36496E-02	-2.29562E-03	-2.84130E-02	-2.05394E-02
14	0.	-1.32850E-02	-3.34188E-02	-4.79448E-02	-6.24782E-02	-7.04060E-02	-5.79607E-02	-2.38100E-02	1.87051E-03	-6.69047E-03
15	0.	2.06533E-02	3.76905E-02	5.36530E-02	6.69531E-02	6.45159E-02	2.68422E-02	-3.74152E-02	-7.17761E-02	-4.56324E-02
16	0.	-2.32440E-02	-4.33357E-02	-6.76649E-02	-9.89494E-02	-.12874	-.12948	-8.77121E-02	-5.12758E-02	-6.84117E-02
17	0.	2.24527E-02	3.88565E-02	5.20470E-02	5.24257E-02	1.26497E-02	-8.44490E-02	-.19435	-.22631	-.16866
18	0.	-4.10785E-02	-7.99358E-02	-.13306	-.23765	-.37401	-.42313	-.32597	-.26011	-.34313
19	0.	6.53433E-02	3.94317E-02	8.99390E-02	9.56842E-03	-.23281	-.55699	-.67802	-.55396	-.50757
20	0.	-.39137	-.46402	-.54055	-.60702	-.74793	-.90269	-.81321	-.69445	-.83764

Table D-1.5

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

MASS FRACTION OF SPECIES, 2, AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	5.43590E-29	2.07514E-28	5.71090E-28	1.12841E-27	1.91086E-27	4.18521E-27
2	0.	0.	0.	0.	5.43590E-29	2.07514E-28	5.71090E-28	1.12841E-27	1.91086E-27	4.18521E-27
3	0.	7.57519E-29	1.25394E-27	9.76458E-27	4.87413E-26	1.71981E-25	4.41658E-25	8.31608E-25	1.14682E-24	1.17460E-24
4	0.	3.36210E-26	4.66790E-25	3.47863E-24	1.71260E-23	5.95892E-23	1.50567E-22	2.78327E-22	3.76034E-22	3.78316E-22
5	0.	1.13753E-23	1.57024E-22	1.16211E-21	5.67477E-21	1.95496E-20	4.87778E-20	8.87066E-20	1.17410E-19	1.15610E-19
6	0.	3.50249E-21	4.78057E-20	3.49606E-19	1.68500E-18	5.71990E-18	1.40327E-17	2.50281E-17	3.24077E-17	3.12468E-17
7	0.	9.83087E-19	1.33249E-17	9.67293E-17	4.62299E-16	1.55337E-15	3.76161E-15	6.59553E-15	8.35751E-15	7.88446E-15
8	0.	2.45140E-16	3.28415E-15	2.35517E-14	1.11068E-13	3.67602E-13	8.74811E-13	1.50329E-12	1.86228E-12	1.72129E-12
9	0.	5.44441E-14	7.16965E-13	5.11962E-12	2.39519E-11	7.85078E-11	1.84512E-10	3.11841E-10	3.78205E-10	3.42567E-10
10	0.	1.01245E-11	1.33357E-10	9.39592E-10	4.34430E-09	1.40485E-08	3.25059E-08	5.39583E-08	6.41451E-08	5.71224E-08
11	0.	1.47202E-10	2.45574E-09	1.72354E-08	7.92596E-08	2.54482E-07	5.83082E-07	9.54719E-07	1.11476E-06	9.76658E-07
12	0.	3.04454E-09	3.95520E-08	2.74354E-07	1.24568E-06	3.94197E-06	8.88460E-06	1.42828E-05	1.63563E-05	1.41252E-05
13	0.	4.13935E-08	5.34116E-07	3.67682E-06	1.65474E-05	5.18152E-05	1.15278E-04	1.82271E-04	2.04516E-04	1.73792E-04
14	0.	4.47274E-07	5.68606E-06	3.84806E-05	1.69823E-04	5.20580E-04	1.13088E-03	1.74311E-03	1.90731E-03	1.59816E-03
15	0.	3.77842E-06	4.71301E-05	3.12600E-04	1.35103E-03	4.04636E-03	8.57486E-03	1.28608E-02	1.36744E-02	1.12957E-02
16	0.	2.45134E-05	2.85687E-04	1.79551E-03	7.39458E-03	2.11515E-02	4.28176E-02	6.12391E-02	6.27083E-02	5.15936E-02
17	0.	1.58350E-04	1.47344E-03	7.80841E-03	2.85537E-02	7.46079E-02	.13803	.17988	.17343	.14981
18	0.	2.02334E-03	1.10157E-02	3.54268E-02	9.08636E-02	.18537	.23569	.19896	.20135	.27507
19	0.	4.38771E-02	.13092	.22327	.30347	.47348	.66021	.55225	.40897	.58172
20	0.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Table D-1.6

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

MASS FRACTION OF SPECIES, 1, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
3	1.0000	1.0000	1.00000	1.00000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
4	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
5	1.0000	1.0000	1.00000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
6	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
7	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
8	1.0000	1.0000	1.00000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000
9	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
10	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
11	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	.99999	.99999	.99998	.99999
13	1.0000	1.00000	1.00000	1.00000	.99998	.99995	.99988	.99982	.99975	.99982
14	1.0000	1.00000	.99999	.99996	.99993	.99947	.99885	.99822	.99805	.99837
15	1.0000	1.00000	.99995	.99958	.99861	.99581	.99106	.98653	.98565	.98829
16	1.0000	.99999	.99970	.99812	.99213	.97705	.95259	.93105	.92980	.94398
17	1.0000	.99934	.99842	.99132	.96656	.90680	.81279	.73868	.75324	.81270
18	1.0000	.99733	.98931	.95829	.87215	.67956	.37766	.19727	.35057	.53134
19	1.0000	.99597	.98027	.74660	.45302	5.05618E-02	0.	8.12394E-02	.15240	1.31023E-02
20	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-1.7

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

MASS FRACTION OF SPECIES, 3, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.	0.	0.	0.	2.17129E-29	1.35076E-28	3.31356E-28	4.80243E-28	5.26427E-28
4	0.	0.	0.93297E-29	9.87746E-28	5.99292E-27	2.45019E-26	7.08202E-26	1.45744E-25	2.10953E-25	2.13670E-25
5	0.	3.04933E-27	4.87506E-26	4.32662E-25	2.52690E-24	1.02207E-23	2.92014E-23	5.89945E-23	8.32260E-23	8.16067E-23
6	0.	1.20243E-24	1.90934E-23	1.67941E-22	9.70262E-22	3.87180E-21	1.09763E-20	2.15078E-20	2.95261E-20	2.80483E-20
7	0.	4.41405E-22	6.98084E-21	6.11492E-20	3.51258E-19	1.38976E-18	3.85470E-18	7.47990E-18	9.99155E-18	9.17148E-18
8	0.	1.47314E-19	2.30331E-18	2.00595E-17	1.14040E-16	4.45355E-16	1.21469E-15	2.30610E-15	2.99320E-15	2.65492E-15
9	0.	4.47343E-17	5.95932E-16	6.05190E-15	3.42587E-14	1.32851E-13	3.58245E-13	6.67851E-13	8.42975E-13	7.21558E-13
10	0.	1.20014E-14	1.86274E-13	1.60227E-12	8.99822E-12	3.45279E-11	9.17833E-11	1.67763E-10	2.05986E-10	1.70380E-10
11	0.	3.26033E-13	5.09174E-12	4.38143E-11	2.45874E-10	9.40405E-10	2.48071E-09	4.46616E-09	5.34066E-09	4.26174E-09
12	0.	8.13633E-12	1.25544E-10	1.07441E-09	5.93931E-09	2.27013E-08	5.91192E-08	1.04445E-07	1.21358E-07	9.32625E-08
13	0.	1.76074E-10	2.74738E-09	2.35374E-08	1.31224E-07	4.96348E-07	1.28413E-06	2.23389E-06	2.51671E-06	1.84891E-06
14	0.	3.41523E-09	5.03021E-08	4.34370E-07	2.40762E-06	9.03299E-06	2.30862E-05	3.93442E-05	4.27132E-05	2.97604E-05
15	0.	5.21055E-08	3.01721E-07	6.87145E-06	3.81516E-05	1.43215E-04	3.64987E-04	6.12679E-04	6.37223E-04	4.13928E-04
16	0.	6.53133E-07	1.00557E-05	8.65489E-05	4.79874E-04	1.80112E-03	4.59792E-03	7.60653E-03	7.46617E-03	4.40456E-03
17	0.	6.31243E-06	9.86532E-05	8.70325E-04	4.90183E-03	1.87144E-02	4.94954E-02	8.15448E-02	7.30322E-02	3.74022E-02
18	0.	4.18023E-05	6.75678E-04	6.30075E-03	3.72432E-02	.13802	.39396	.60466	.44355	.19585
19	0.	1.57954E-04	2.81301E-03	3.02671E-02	.24642	.52100	.46640	.32085	.42655	.44950
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-I.8

CALCULATED VALUES AT L = 1001, IT = 3 TIME = 3.0518E-03 SEC.

TEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3143.6	3125.9	3125.7	3125.7	3125.7	3125.7	3125.7	3125.7	3125.7	3125.7
3	3047.8	3029.5	3029.2	3029.2	3029.2	3029.2	3029.2	3029.2	3029.2	3029.2
4	2952.4	2934.2	2933.9	2933.9	2933.9	2933.9	2933.9	2933.9	2933.9	2933.9
5	2857.4	2838.3	2838.6	2838.6	2838.6	2838.6	2838.6	2838.6	2838.6	2838.6
6	2763.0	2738.7	2738.3	2738.3	2738.3	2738.3	2738.3	2738.3	2738.3	2738.3
7	2663.0	2602.3	2601.4	2601.4	2601.4	2601.4	2601.4	2601.4	2601.4	2601.4
8	2389.7	2338.2	2337.5	2337.5	2337.5	2337.5	2337.5	2337.5	2337.5	2337.5
9	2114.3	2065.0	2064.3	2064.3	2064.3	2064.3	2064.3	2064.3	2064.3	2064.3
10	1842.9	1794.3	1794.3	1794.2	1794.2	1794.2	1794.2	1794.2	1794.2	1794.2
11	1575.2	1526.5	1527.9	1527.9	1527.9	1527.9	1527.9	1527.9	1527.9	1527.9
12	1311.1	1265.3	1265.1	1265.1	1265.1	1265.1	1265.1	1265.1	1265.1	1265.1
13	1050.7	1006.9	1006.3	1006.3	1006.3	1006.3	1006.3	1006.3	1006.3	1006.3
14	793.64	755.83	755.33	755.33	755.33	755.33	755.33	755.33	755.33	755.33
15	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

Table D-2.1 - D-2.8 Computed Results for All the Dependent Variables at $t \approx 0.006$ Sec with Modified Values for the Reaction Orders

Table D-2.1

CALCULATED VALUES AT L = 1001. IT = 2 TIME = 6.1035E-03 SEC.

DENSITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.13500	.13369	.13238	.13108	.12979	.12850	.12723	.12597	.12483	.12413
2	.13500	.13369	.13238	.13108	.12979	.12850	.12723	.12597	.12483	.12413
3	.13500	.13447	.13393	.13340	.13286	.13232	.13178	.13124	.13082	.13087
4	.13500	.13383	.13267	.13150	.13034	.12919	.12803	.12689	.12586	.12527
5	.13500	.13451	.13402	.13355	.13308	.13261	.13216	.13172	.13141	.13158
6	.13500	.13385	.13269	.13153	.13036	.12919	.12801	.12684	.12578	.12515
7	.13500	.13449	.13400	.13353	.13307	.13262	.13219	.13179	.13153	.13176
8	.13500	.13383	.13265	.13146	.13025	.12903	.12780	.12657	.12545	.12476
9	.13500	.13445	.13392	.13341	.13292	.13246	.13202	.13162	.13138	.13167
10	.13500	.13364	.13227	.13090	.12953	.12815	.12677	.12539	.12413	.12332
11	.13500	.13441	.13385	.13330	.13277	.13226	.13177	.13132	.13104	.13130
12	.13500	.13363	.13223	.13082	.12940	.12797	.12653	.12509	.12376	.12287
13	.13500	.13438	.13379	.13323	.13269	.13217	.13168	.13120	.13084	.13093
14	.13500	.13360	.13217	.13072	.12924	.12775	.12621	.12458	.12285	.12119
15	.13500	.13433	.13371	.13312	.13254	.13195	.13125	.13017	.12836	.12563
16	.13500	.13355	.13206	.13054	.12895	.12719	.12491	.12134	.11566	.10787
17	.13500	.13425	.13355	.13284	.13202	.13061	.12712	.11966	.10846	9.66726E-02
18	.13500	.13341	.13164	.12965	.12713	.12245	.10988	9.42517E-02	8.33088E-02	8.01193E-02
19	.13500	.13305	.13036	.12798	.12477	.11487	7.39668E-02	8.82869E-02	7.73955E-02	6.55600E-02
20	.13500	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382

Table D-2.2

CALCULATED VALUES AT L = 1301, IT = 2 TIME = 6.1035E-03 SEC.

GAS PHASE TEMPERATURE AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	3240.0	3271.9	3304.2	3336.9	3370.1	3403.8	3437.9	3472.5	3508.3	3553.2
2	3240.0	3271.9	3304.2	3336.9	3370.1	3403.8	3437.9	3472.5	3508.3	3553.2
3	3240.0	3252.8	3265.8	3278.9	3292.2	3305.6	3319.2	3333.0	3347.8	3371.5
4	3240.0	3268.2	3296.9	3326.1	3355.7	3385.8	3416.4	3447.5	3479.8	3521.1
5	3240.0	3251.8	3263.6	3275.2	3286.8	3298.3	3309.7	3321.0	3333.0	3353.5
6	3240.0	3267.8	3296.3	3325.5	3355.3	3385.7	3416.9	3448.7	3481.9	3524.2
7	3240.0	3252.2	3264.1	3275.8	3287.1	3298.1	3308.9	3319.2	3330.0	3348.8
8	3240.0	3268.2	3297.4	3327.3	3358.2	3389.9	3422.5	3456.1	3491.1	3535.2
9	3240.0	3253.3	3266.2	3278.6	3290.6	3302.1	3313.1	3323.4	3333.7	3351.3
10	3240.0	3273.0	3306.8	3341.4	3376.8	3413.2	3450.5	3488.6	3528.0	3576.1
11	3240.0	3254.1	3267.9	3281.4	3294.5	3307.2	3319.4	3330.9	3342.2	3360.5
12	3240.0	3273.3	3307.8	3343.4	3380.1	3418.0	3457.0	3497.0	3538.6	3589.0
13	3240.0	3254.9	3269.2	3283.0	3296.4	3309.3	3321.8	3334.1	3347.3	3369.5
14	3240.0	3274.0	3309.4	3346.2	3384.3	3424.0	3465.8	3511.3	3564.6	3637.8
15	3240.0	3256.1	3271.3	3285.9	3300.1	3314.7	3332.4	3360.1	3411.4	3509.6
16	3240.0	3275.1	3312.0	3350.7	3391.9	3438.6	3501.3	3604.6	3787.7	4091.5
17	3240.0	3258.0	3274.9	3291.7	3311.1	3345.7	3438.6	3662.8	4076.0	4683.2
18	3240.0	3277.4	3317.5	3361.2	3418.8	3544.2	3978.6	4765.7	5640.8	6620.8
19	3240.0	3261.0	3278.3	3297.0	3347.8	3639.6	6323.4	6840.0	6840.0	6577.9
20	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0

Table D-2.3

CALCULATED VALUES AT L = 1001, IT = 2 TIME = 6.1035E-03 SEC.

Z-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000
2	19.746	19.775	19.806	19.838	19.871	19.905	19.940	19.977	20.014	20.053
3	19.470	19.477	19.484	19.489	19.493	19.496	19.498	19.498	19.497	19.495
4	19.168	19.200	19.232	19.266	19.301	19.338	19.377	19.417	19.459	19.503
5	18.936	18.844	18.851	18.857	18.862	18.865	18.866	18.866	18.864	18.860
6	18.463	18.495	18.528	18.563	18.600	18.638	18.678	18.720	18.764	18.810
7	18.040	18.049	18.057	18.064	18.069	18.072	18.074	18.074	18.072	18.066
8	17.546	17.578	17.612	17.647	17.685	17.724	17.765	17.808	17.854	17.902
9	16.952	16.966	16.980	16.991	17.002	17.010	17.017	17.021	17.023	17.020
10	16.723	16.775	16.826	16.877	16.928	16.979	17.031	17.083	17.138	17.194
11	16.473	16.466	16.460	16.456	16.453	16.450	16.447	16.443	16.436	16.423
12	16.198	16.246	16.293	16.341	16.388	16.435	16.483	16.533	16.584	16.640
13	15.892	15.888	15.884	15.880	15.876	15.871	15.866	15.859	15.849	15.830
14	15.546	15.538	15.631	15.677	15.723	15.769	15.816	15.864	15.914	15.971
15	15.146	15.147	15.144	15.139	15.132	15.124	15.115	15.103	15.085	15.050
16	14.671	14.701	14.736	14.773	14.811	14.846	14.877	14.900	14.913	14.926
17	14.080	14.077	14.061	14.030	13.983	13.918	13.826	13.690	13.481	13.192
18	13.288	13.242	13.143	13.005	12.829	12.601	12.269	11.759	11.082	10.470
19	12.035	11.144	10.331	9.5816	8.8700	8.1150	7.1293	5.9255	4.8073	4.1738
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-2.4

CALCULATED VALUES AT L = 1001, IT = 2 TIME = 6.1035E-03 SEC.

R-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	-1.06011E-03	-2.15773E-03	-3.32820E-03	-4.54336E-03	-5.81480E-03	-7.14187E-03	-8.51477E-03	-9.89404E-03	-1.11734E-02
3	0.	1.31594E-03	2.69957E-03	4.16635E-03	5.71881E-03	7.35959E-03	9.08872E-03	1.08949E-02	1.27288E-02	1.44458E-02
4	0.	-1.90891E-03	-3.92041E-03	-6.06216E-03	-8.33817E-03	-1.07530E-02	-1.33077E-02	-1.59878E-02	-1.87218E-02	-2.12884E-02
5	0.	2.26144E-03	4.65031E-03	7.23754E-03	9.99854E-03	1.29501E-02	1.60964E-02	1.94249E-02	2.28560E-02	2.61115E-02
6	0.	-2.80933E-03	-5.79585E-03	-9.01492E-03	-1.24741E-02	-1.61836E-02	-2.01518E-02	-2.43698E-02	-2.87465E-02	-3.29232E-02
7	0.	3.20574E-03	6.62892E-03	1.03403E-02	1.43493E-02	1.86700E-02	2.33179E-02	2.82951E-02	3.35130E-02	3.85437E-02
8	0.	-3.71150E-03	-7.68325E-03	-1.20031E-02	-1.66839E-02	-2.17456E-02	-2.72145E-02	-3.31108E-02	-3.93563E-02	-4.54413E-02
9	0.	4.22492E-03	8.71728E-03	1.35913E-02	1.88690E-02	2.45819E-02	3.07756E-02	3.75022E-02	4.47091E-02	5.17877E-02
10	0.	-6.49388E-03	-1.26880E-02	-1.88982E-02	-2.52807E-02	-3.19704E-02	-3.91107E-02	-4.68807E-02	-5.53806E-02	-6.39424E-02
11	0.	9.21282E-03	1.72656E-02	2.47271E-02	3.19685E-02	3.92827E-02	4.69500E-02	5.53053E-02	6.46033E-02	7.40169E-02
12	0.	-1.24430E-02	-2.27686E-02	-3.18450E-02	-4.02841E-02	-4.85622E-02	-5.71521E-02	-6.66845E-02	-7.78419E-02	-8.98966E-02
13	0.	1.53516E-02	2.76667E-02	3.81024E-02	4.74654E-02	5.63778E-02	6.54548E-02	7.55211E-02	8.74250E-02	9.99189E-02
14	0.	-1.82126E-02	-3.20776E-02	-4.48139E-02	-5.55722E-02	-6.57377E-02	-7.62567E-02	-8.87470E-02	-.10548	-.12620
15	0.	2.05900E-02	3.68268E-02	5.02496E-02	6.17543E-02	7.20291E-02	8.18013E-02	9.22275E-02	.10468	.11689
16	0.	-2.31342E-02	-4.21146E-02	-5.67540E-02	-7.39538E-02	-8.88141E-02	-.10581	-.13046	-.17059	-.22601
17	0.	2.24943E-02	3.92329E-02	5.05994E-02	6.05658E-02	6.76816E-02	6.94530E-02	6.30525E-02	5.06263E-02	4.03283E-02
18	0.	-4.39557E-02	-7.39539E-02	-9.71262E-02	-.11720	-.13927	-.17640	-.24894	-.38319	-.56168
19	0.	6.45703E-02	8.43596E-02	8.74842E-02	8.20092E-02	7.54890E-02	6.30287E-02	1.11916E-02	-.11793	-.22547
20	0.	-.39157	-.46003	-.51923	-.57198	-.61701	-.61021	-.60510	-.78843	-.94796

Table D-2.5

CALCULATED VALUES AT L = 1001, IT = 2 TIME = 6.1035E-03 SEC.

MASS FRACTION OF SPECIES, 2, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	7.75862E-29	6.88185E-28	4.46655E-27	2.35105E-26	1.02817E-25	3.78144E-25	1.16786E-24
2	0.	0.	0.	7.75862E-29	6.88185E-28	4.46655E-27	2.35105E-26	1.02817E-25	3.78144E-25	1.16786E-24
3	0.	1.92904E-28	3.36271E-27	3.59374E-26	2.87834E-25	1.83414E-24	9.56211E-24	4.14056E-23	1.50072E-22	4.50050E-22
4	0.	3.73612E-26	6.44118E-25	6.81760E-24	5.39471E-23	3.39362E-22	1.74530E-21	7.44893E-21	2.65856E-20	7.84984E-20
5	0.	6.80646E-24	1.16543E-22	1.22457E-21	9.61499E-21	5.99789E-20	3.05649E-19	1.29140E-18	4.55785E-18	1.32957E-17
6	0.	1.13135E-21	1.91390E-20	1.99563E-19	1.53863E-18	9.46639E-18	4.75400E-17	1.97753E-16	6.86401E-16	1.96864E-15
7	0.	1.72584E-19	2.89537E-18	2.97859E-17	2.28788E-16	1.39450E-15	6.93260E-15	2.85198E-14	9.77898E-14	2.76764E-13
8	0.	2.34357E-17	3.87784E-16	3.93288E-15	2.97690E-14	1.78693E-13	8.74132E-13	3.53478E-12	1.18992E-11	3.30505E-11
9	0.	2.83100E-15	4.63595E-14	4.65322E-13	3.48530E-12	2.06951E-11	1.00086E-10	3.99800E-10	1.32809E-09	3.63620E-09
10	0.	2.91472E-13	4.69640E-12	4.63203E-11	3.40852E-10	1.98841E-09	9.44544E-09	3.70369E-08	1.20656E-07	3.23923E-07
11	0.	3.19390E-12	5.06069E-11	4.89952E-10	3.54382E-09	2.03596E-08	9.53728E-08	3.68955E-07	1.18546E-06	3.13681E-06
12	0.	3.54950E-11	5.37731E-10	4.96226E-09	3.44170E-08	1.91048E-07	8.69569E-07	3.27860E-06	1.02784E-05	2.65654E-05
13	0.	4.25276E-10	5.87339E-09	4.91020E-08	3.13914E-07	1.64311E-06	7.17791E-06	2.62518E-05	8.02457E-05	2.02700E-04
14	0.	6.40387E-09	7.46867E-08	5.11565E-07	2.72806E-06	1.24473E-05	4.94799E-05	1.69486E-04	4.92729E-04	1.19358E-03
15	0.	1.29041E-07	1.24267E-06	6.63792E-06	2.70505E-05	9.73110E-05	3.25188E-04	9.94447E-04	2.68150E-03	6.14573E-03
16	0.	2.99832E-06	2.37448E-05	9.91349E-05	3.01779E-04	7.92859E-04	1.98988E-03	4.90694E-03	1.14470E-02	2.36934E-02
17	0.	7.34845E-05	4.66631E-04	1.52540E-03	3.57695E-03	7.06991E-03	1.30393E-02	2.42291E-02	4.60311E-02	8.14772E-02
18	0.	1.79516E-03	8.38289E-03	2.01136E-02	3.56808E-02	5.44065E-02	7.49433E-02	.10322	.16099	.22317
19	0.	4.35177E-02	.12611	.19755	.26119	.31552	.30732	.30115	.52235	.71483
20	0.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Table D-2.6

CALCULATED VALUES AT L = 1001, IT = 2 TIME = 6.1035E-03 SEC.

MASS FRACTION OF SPECIES, 1, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.00000
3	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.0000
4	1.0000	1.0000	1.0000	1.00000	1.00000	1.0000	1.00000	1.0000	1.00000	1.00000
5	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
10	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
11	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	.99999	.99997
13	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	.99999	.99997	.99991	.99978
14	1.0000	1.00000	1.00000	1.00000	1.00000	.99999	.99995	.99981	.99946	.99867
15	1.0000	1.00000	1.00000	.99999	.99997	.99990	.99964	.99885	.99683	.99259
16	1.0000	1.00000	.99998	.99990	.99969	.99914	.99769	.99386	.98479	.96689
17	1.0000	.99993	.99953	.99847	.99635	.99243	.98435	.96610	.92688	.85393
18	1.0000	.99820	.99161	.97984	.96386	.94224	.90522	.82875	.68694	.44818
19	1.0000	.95648	.87387	.80224	.73670	.66617	.51302	.19996	0.	0.
20	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-2.7

CALCULATED VALUES AT L = 1001, IT = 2 TIME = 6.1035E-03 SEC.

MASS FRACTION OF SPECIES, 3, AT GRID POINT(M,N)

N= M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	3.70952E-29	2.05852E-28	1.15637E-27	7.96086E-27
2	0.	0.	0.	0.	0.	0.	3.70952E-29	2.05852E-28	1.15637E-27	7.96086E-27
3	0.	0.	0.	0.	6.09266E-28	4.54916E-27	2.55452E-26	1.18158E-25	4.55242E-25	1.43434E-24
4	0.	9.51780E-29	1.68488E-27	1.86114E-26	1.55017E-25	1.03838E-24	5.70943E-24	2.60471E-23	9.90153E-23	3.08779E-22
5	0.	2.13244E-26	3.74226E-25	4.10215E-24	3.40745E-23	2.26854E-22	1.23849E-21	5.60390E-21	2.10996E-20	6.50882E-20
6	0.	4.41401E-24	7.65180E-23	8.30816E-22	6.82634E-21	4.49325E-20	2.42315E-19	1.08177E-18	4.01308E-18	1.21893E-17
7	0.	8.51732E-22	1.46862E-20	1.58308E-19	1.29318E-18	8.45857E-18	4.52885E-17	2.00486E-16	7.36408E-16	2.21136E-15
8	0.	1.49271E-19	2.54411E-18	2.71232E-17	2.19142E-16	1.41687E-15	7.49055E-15	3.26951E-14	1.18216E-13	3.49124E-13
9	0.	2.38017E-17	4.02957E-16	4.27264E-15	3.43415E-14	2.20762E-13	1.15914E-12	5.01782E-12	1.79636E-11	5.24377E-11
10	0.	3.32509E-15	5.57437E-14	5.85564E-13	4.66213E-12	2.96617E-11	1.53912E-10	6.57232E-10	2.31637E-09	6.64988E-09
11	0.	4.87812E-14	8.15349E-13	8.55610E-12	6.80051E-11	4.31495E-10	2.22903E-09	9.45593E-09	3.30367E-08	9.38307E-08
12	0.	6.70406E-13	1.12153E-11	1.16667E-10	9.19726E-10	5.78100E-09	2.95127E-08	1.23365E-07	4.23542E-07	1.18066E-06
13	0.	8.47903E-12	1.40207E-10	1.45747E-09	1.14887E-08	7.21146E-08	3.66423E-07	1.51799E-06	5.14651E-06	1.41358E-05
14	0.	9.30973E-11	1.52759E-09	1.57932E-08	1.23937E-07	7.73148E-07	3.88222E-06	1.57723E-05	5.21353E-05	1.39416E-04
15	0.	9.03998E-10	1.46327E-08	1.54203E-07	1.22072E-06	7.67426E-06	3.84941E-05	1.54026E-04	4.96587E-04	1.29401E-03
16	0.	7.40646E-09	1.21319E-07	1.26996E-06	1.01876E-05	6.49634E-05	3.26191E-04	1.26791E-03	3.89681E-03	9.73910E-03
17	0.	5.09935E-08	8.46120E-07	9.12307E-06	7.63909E-05	5.12092E-04	2.67577E-03	1.00855E-02	2.87824E-02	6.85555E-02
18	0.	2.67590E-07	4.35884E-06	5.17008E-05	4.64806E-04	3.41621E-03	2.04404E-02	7.22076E-02	.17077	.36734
19	0.	9.19470E-07	1.68742E-05	2.11384E-04	2.14037E-03	1.87128E-02	.18371	.53266	.65861	.54249
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-2.8

CALCULATED VALUES AT I = 1001, IT = 2 TIME = 6.1035E-03 SEC.

TEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3143.6	3110.0	3109.1	3109.1	3109.1	3109.1	3109.1	3109.1	3109.1	3109.1
3	3047.8	3011.7	3010.8	3010.7	3010.7	3010.7	3010.7	3010.7	3010.7	3010.7
4	2952.4	2916.1	2915.1	2915.1	2915.1	2915.1	2915.1	2915.1	2915.1	2915.1
5	2857.4	2818.2	2817.1	2817.1	2817.1	2817.1	2817.1	2817.1	2817.1	2817.1
6	2763.0	2706.3	2704.6	2704.6	2704.6	2704.6	2704.6	2704.6	2704.6	2704.6
7	2669.0	2544.0	2540.7	2540.7	2540.7	2540.7	2540.7	2540.7	2540.7	2540.7
8	2389.7	2287.7	2284.9	2284.8	2284.8	2284.8	2284.8	2284.8	2284.8	2284.8
9	2114.3	2017.1	2014.4	2014.4	2014.4	2014.4	2014.4	2014.4	2014.4	2014.4
10	1842.9	1748.4	1745.9	1745.8	1745.8	1745.8	1745.8	1745.8	1745.8	1745.8
11	1575.2	1483.3	1480.9	1480.8	1480.8	1480.8	1480.8	1480.8	1480.8	1480.8
12	1311.1	1222.1	1219.7	1219.7	1219.7	1219.7	1219.7	1219.7	1219.7	1219.7
13	1050.7	966.66	964.43	964.39	964.39	964.39	964.39	964.39	964.39	964.39
14	793.64	727.24	725.60	725.57	725.57	725.57	725.57	725.57	725.57	725.57
15	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00

NOTE MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

Table D-3.1 - D-3.8 Computed Results for All the Dependent Variables at $t \simeq 0.009$ Sec with Modified Values for the Reaction Orders

Table D-3.1

CALCULATED VALUES AT L = 1001, IT = 1

TIME = 9.1553E-03 SEC.

DENSITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	.13500	.13369	.13238	.13108	.12979	.12850	.12723	.12596	.12470	.12305
2	.13500	.13369	.13238	.13108	.12979	.12850	.12723	.12596	.12470	.12305
3	.13500	.13447	.13393	.13340	.13286	.13232	.13178	.13123	.13068	.12969
4	.13500	.13383	.13267	.13150	.13034	.12919	.12803	.12688	.12572	.12417
5	.13500	.13451	.13402	.13355	.13308	.13261	.13216	.13171	.13126	.13038
6	.13500	.13385	.13269	.13153	.13036	.12919	.12801	.12683	.12564	.12406
7	.13500	.13449	.13400	.13353	.13307	.13262	.13219	.13177	.13137	.13055
8	.13500	.13383	.13265	.13146	.13025	.12903	.12780	.12656	.12530	.12366
9	.13500	.13445	.13392	.13341	.13292	.13246	.13202	.13160	.13121	.13042
10	.13500	.13364	.13227	.13090	.12953	.12815	.12676	.12537	.12397	.12220
11	.13500	.13441	.13385	.13330	.13277	.13226	.13177	.13130	.13085	.13002
12	.13500	.13363	.13223	.13082	.12940	.12797	.12652	.12507	.12360	.12177
13	.13500	.13438	.13379	.13323	.13269	.13217	.13168	.13121	.13076	.12993
14	.13500	.13360	.13217	.13072	.12925	.12776	.12626	.12474	.12320	.12128
15	.13500	.13433	.13371	.13312	.13255	.13202	.13150	.13099	.13045	.12942
16	.13500	.13355	.13206	.13054	.12899	.12742	.12580	.12408	.12209	.11923
17	.13500	.13425	.13355	.13287	.13220	.13152	.13074	.12935	.12630	.12080
18	.13500	.13341	.13165	.12974	.12772	.12556	.12276	.11587	.10345	9.26517E-02
19	.13500	.13306	.13039	.12820	.12638	.12458	.11946	9.22932E-02	7.61001E-02	9.90507E-02
20	.13500	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382	.11382

Table D-3.2

CALCULATED VALUES AT I = 1001, IT = 1

TIME = 9.1553E-03 SEC.

GAS PHASE TEMPERATURE AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	3240.0	3271.9	3304.2	3336.9	3370.1	3403.8	3437.9	3472.5	3507.0	3527.3
2	3240.0	3271.9	3304.2	3336.9	3370.1	3403.8	3437.9	3472.5	3507.0	3527.3
3	3240.0	3252.8	3265.8	3278.9	3292.2	3305.6	3319.2	3333.0	3346.4	3345.2
4	3240.0	3268.2	3296.9	3326.1	3355.7	3385.8	3416.4	3447.4	3478.5	3495.0
5	3240.0	3251.8	3263.6	3275.2	3286.8	3298.3	3309.7	3321.0	3331.7	3327.2
6	3240.0	3267.8	3296.3	3325.5	3355.3	3385.7	3416.9	3448.7	3480.7	3498.3
7	3240.0	3252.2	3264.1	3275.8	3287.1	3298.1	3308.9	3319.3	3328.9	3322.9
8	3240.0	3268.2	3297.4	3327.3	3358.2	3389.9	3422.6	3456.2	3490.2	3509.8
9	3240.0	3253.3	3266.2	3278.6	3290.6	3302.1	3313.1	3323.6	3333.1	3326.4
10	3240.0	3273.0	3306.8	3341.4	3376.8	3413.2	3450.5	3488.8	3527.7	3552.0
11	3240.0	3254.1	3267.9	3281.4	3294.5	3307.2	3319.5	3331.3	3342.1	3336.8
12	3240.0	3273.3	3307.8	3343.4	3380.1	3418.0	3457.0	3497.2	3538.1	3564.7
13	3240.0	3254.5	3269.2	3283.0	3296.4	3309.3	3321.7	3333.6	3344.5	3336.3
14	3240.0	3274.0	3309.4	3346.2	3384.3	3423.7	3464.4	3506.5	3549.8	3579.5
15	3240.0	3256.1	3271.3	3285.8	3299.8	3313.2	3326.2	3339.0	3352.2	3352.5
16	3240.0	3275.1	3312.0	3350.6	3390.7	3432.4	3476.2	3523.9	3580.8	3641.0
17	3240.0	3258.0	3274.9	3291.0	3306.6	3321.9	3339.4	3373.2	3455.5	3597.1
18	3240.0	3277.4	3317.2	3358.9	3402.4	3449.4	3516.8	3727.1	4230.0	4844.5
19	3240.0	3260.9	3277.7	3290.8	3300.7	3315.2	3438.7	4621.6	6840.0	6840.0
20	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0

Table D-3.3

CALCULATED VALUES AT L = 1001, IT = 1

TIME = 9.1553E-03 SEC.

Z-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000	20.000
2	19.746	19.775	19.806	19.838	19.871	19.905	19.940	19.977	20.015	20.054
3	19.470	19.477	19.484	19.489	19.493	19.496	19.498	19.498	19.497	19.495
4	19.168	19.200	19.232	19.266	19.301	19.338	19.377	19.417	19.459	19.503
5	18.836	18.844	18.851	18.857	18.862	18.865	18.866	18.866	18.864	18.861
6	18.463	18.495	18.528	18.563	18.600	18.638	18.678	18.720	18.764	18.810
7	18.040	18.049	18.057	18.064	18.069	18.072	18.074	18.074	18.073	18.069
8	17.545	17.578	17.612	17.647	17.685	17.724	17.765	17.808	17.854	17.901
9	16.952	16.966	16.980	16.991	17.002	17.010	17.017	17.022	17.025	17.026
10	16.723	16.775	16.826	16.877	16.928	16.979	17.031	17.083	17.137	17.193
11	16.473	16.466	16.460	16.456	16.453	16.450	16.447	16.443	16.439	16.433
12	16.198	16.246	16.294	16.341	16.388	16.435	16.484	16.533	16.584	16.637
13	15.892	15.888	15.884	15.880	15.876	15.871	15.866	15.859	15.852	15.843
14	15.546	15.588	15.631	15.677	15.723	15.770	15.818	15.866	15.917	15.968
15	15.146	15.147	15.144	15.139	15.132	15.124	15.113	15.102	15.087	15.069
16	14.671	14.701	14.736	14.773	14.811	14.848	14.883	14.915	14.942	14.963
17	14.080	14.077	14.061	14.030	13.984	13.923	13.845	13.749	13.626	13.462
18	13.298	13.242	13.144	13.006	12.836	12.639	12.415	12.150	11.806	11.338
19	12.035	11.144	10.331	9.5856	8.8970	8.2531	7.6268	6.9227	6.0705	5.1423
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-3.4

CALCULATED VALUES AT L = 1001, TT = 1 TIME = 9.1553E-03 SEC.

R-VELOCITY AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	-1.06011E-03	-2.16774E-03	-3.32822E-03	-4.54350E-03	-5.81575E-03	-7.14722E-03	-8.54025E-03	-9.99687E-03	-1.15102E-02
3	0.	1.31594E-03	2.69957E-03	4.16636E-03	5.71893E-03	7.36052E-03	9.09449E-03	1.09243E-02	1.28526E-02	1.48555E-02
4	0.	-1.60891E-03	-3.52041E-03	-6.06216E-03	-8.33825E-03	-1.07539E-02	-1.33144E-02	-1.60256E-02	-1.88917E-02	-2.18765E-02
5	0.	2.26144E-03	4.66031E-03	7.23749E-03	9.99837E-03	1.29500E-02	1.60996E-02	1.94547E-02	2.30211E-02	2.67451E-02
6	0.	-2.30939E-03	-5.79584E-03	-9.01482E-03	-1.24736E-02	-1.61818E-02	-2.01494E-02	-2.43871E-02	-2.89028E-02	-3.36243E-02
7	0.	3.20574E-03	6.62889E-03	1.03400E-02	1.43430E-02	1.86648E-02	2.33028E-02	2.82748E-02	3.35911E-02	3.91585E-02
8	0.	-3.71150E-03	-7.68321E-03	-1.20028E-02	-1.66817E-02	-2.17355E-02	-2.71802E-02	-3.30327E-02	-3.93070E-02	-4.58897E-02
9	0.	4.22402E-03	8.71722E-03	1.35907E-02	1.88652E-02	2.45638E-02	3.07092E-02	3.73245E-02	4.44288E-02	5.18893E-02
10	0.	-4.49389E-03	-1.26879E-02	-1.88975E-02	-2.52750E-02	-3.19385E-02	-3.89783E-02	-4.64648E-02	-5.44515E-02	-6.27714E-02
11	0.	9.21285E-03	1.72657E-02	2.47268E-02	3.19630E-02	3.92426E-02	4.67613E-02	5.46630E-02	6.30512E-02	7.17440E-02
12	0.	-1.24430E-02	-2.27690E-02	-3.18461E-02	-4.02805E-02	-4.85096E-02	-5.68512E-02	-6.55371E-02	-7.47370E-02	-8.42684E-02
13	0.	1.53517E-02	2.76678E-02	3.81070E-02	4.74740E-02	5.63500E-02	6.51589E-02	7.42061E-02	8.37075E-02	9.34396E-02
14	0.	-1.82129E-02	-3.26797E-02	-4.48234E-02	-5.55922E-02	-6.56902E-02	-7.56531E-02	-8.58887E-02	-9.67375E-02	-.10805
15	0.	2.05903E-02	3.68311E-02	5.02752E-02	6.18538E-02	7.22848E-02	8.21371E-02	9.18224E-02	.10156	.11078
16	0.	-2.31345E-02	-4.21196E-02	-5.87773E-02	-7.39697E-02	-8.83660E-02	-.10257	-.11722	-.13334	-.15210
17	0.	2.24947E-02	3.82422E-02	5.06983E-02	6.11864E-02	7.05367E-02	7.92128E-02	8.69072E-02	9.22713E-02	9.20822E-02
18	0.	-4.39587E-02	-7.39563E-02	-9.73612E-02	-.11770	-.13731	-.15775	-.18149	-.20926	-.24239
19	0.	6.46511E-02	8.42000E-02	8.64879E-02	7.74240E-02	6.25154E-02	4.89893E-02	4.49580E-02	5.64340E-02	6.13835E-02
20	0.	-.33157	-.46002	-.51920	-.57197	-.61952	-.65995	-.66584	-.59150	-.55911

Table D-3.5

CALCULATED VALUES AT L = 1001. TT = 1 TIME = 9.1553E-03 SEC.

MASS FRACTION OF SPECIES. 2. AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	9.08252E-30	9.78103E-29	7.92673E-28	5.42990E-27	3.22891E-26	1.67943E-25	7.50756E-25
2	0.	0.	0.	9.08252E-30	9.78103E-29	7.92673E-28	5.42990E-27	3.22891E-26	1.67943E-25	7.50756E-25
3	0.	1.41470E-29	2.64046E-28	3.17031E-27	2.99696E-26	2.36538E-25	1.60139E-24	9.42856E-24	4.83607E-23	2.05784E-22
4	0.	2.01598E-27	3.71333E-26	4.40588E-25	4.10336E-24	3.18945E-23	2.12658E-22	1.23322E-21	6.23200E-21	2.61727E-20
5	0.	2.76943E-25	5.04475E-24	5.90859E-23	5.42945E-22	4.16504E-21	2.74234E-20	1.57123E-19	7.84740E-19	3.25763E-18
6	0.	3.60243E-23	6.42378E-22	7.33816E-21	6.57315E-20	4.92148E-19	3.16863E-18	1.77846E-17	8.71548E-17	3.56051E-16
7	0.	4.63918E-21	8.05071E-20	8.89385E-19	7.70048E-18	5.59108E-17	3.50703E-16	1.92602E-15	9.26585E-15	3.72419E-14
8	0.	6.10933E-19	1.00870E-17	1.04593E-16	8.48028E-16	5.80016E-15	3.46050E-14	1.82522E-13	8.50125E-13	3.33412E-12
9	0.	8.97414E-17	1.38759E-15	1.31499E-14	9.65465E-14	6.01285E-13	3.31759E-12	1.64839E-11	7.34995E-11	2.79300E-10
10	0.	1.49629E-14	2.13395E-13	1.79893E-12	1.14682E-11	6.15543E-11	2.96080E-10	1.31526E-09	5.39824E-09	1.94197E-08
11	0.	3.27832E-13	4.35822E-12	3.31092E-11	1.84721E-10	8.48417E-10	3.46578E-09	1.32600E-08	4.83774E-08	1.60633E-07
12	0.	7.95806E-12	9.70712E-11	6.66055E-10	3.27773E-09	1.29647E-08	4.46358E-08	1.42715E-07	4.42085E-07	1.29984E-06
13	0.	1.94474E-10	2.22017E-09	1.37911E-08	6.04733E-08	2.09743E-07	6.20848E-07	1.67221E-06	4.33091E-06	1.09073E-05
14	0.	4.80183E-09	4.96258E-08	2.73541E-07	1.05332E-06	3.18387E-06	8.12806E-06	1.85577E-05	3.99404E-05	8.37645E-05
15	0.	1.19637E-07	1.09779E-06	5.28153E-06	1.76700E-05	4.64692E-05	1.03349E-04	2.04541E-04	3.76022E-04	6.66011E-04
16	0.	2.95529E-06	2.30860E-05	9.31238E-05	2.61525E-04	5.82985E-04	1.11116E-03	1.89306E-03	2.97237E-03	4.44541E-03
17	0.	7.33247E-05	4.64256E-04	1.50428E-03	3.44138E-03	6.40569E-03	1.04357E-02	1.53734E-02	2.07533E-02	2.65176E-02
18	0.	1.79478E-03	8.37719E-03	2.00649E-02	3.54027E-02	5.33723E-02	7.28840E-02	9.05517E-02	.10014	.10540
19	0.	4.35177E-02	.12610	.19751	.26117	.31854	.36733	.37443	.28475	.24566
20	0.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Table D-3.6

CALCULATED VALUES AT L = 1001, IT = 1 TIME = 9.1553E-03 SEC.

MASS FRACTION OF SPECIES, 1, AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
3	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
4	1.0000	1.0000	1.0000	1.00000	1.00000	1.0000	1.00000	1.00000	1.00000	1.00000
5	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	1.0000	1.00000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	1.0000	1.00000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
10	1.0000	1.0000	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
11	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
13	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	.99995
14	1.0000	1.00000	1.00000	1.00000	1.00000	1.00000	.99999	.99998	.99996	.99991
15	1.0000	1.00000	1.00000	.99999	.99998	.99995	.99990	.99979	.99960	.99923
16	1.0000	1.00000	.99998	.99991	.99974	.99942	.99888	.99805	.99677	.99468
17	1.0000	.99993	.99954	.99850	.99656	.99359	.98949	.98407	.97652	.96483
18	1.0000	.99821	.99162	.97993	.96459	.94657	.92647	.90353	.87156	.81951
19	1.0000	.95648	.87390	.80249	.73880	.68111	.62745	.56090	.40345	.16029
20	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-3.7

CALCULATED VALUES AT L = 1001. IT = 1 TIME = 9.1553E-03 SEC.

MASS FRACTION OF SPECIES. 3. AT GRID POINT(M,N)

N= / M	1	2	3	4	5	6	7	8	9	10
1	0.	0.	0.	0.	0.	0.	3.37752E-29	2.44661E-28	1.34697E-27	5.58052E-27
2	0.	0.	0.	0.	0.	0.	3.37752E-29	2.44661E-28	1.34697E-27	5.58052E-27
3	0.	0.	0.	0.	2.20611E-23	2.04147E-27	1.45163E-26	8.87106E-26	4.71108E-25	2.06416E-24
4	0.	1.95432E-22	3.65688E-28	4.42176E-27	4.20557E-26	3.37215E-25	2.32971E-24	1.40259E-23	7.35372E-23	3.18586E-22
5	0.	3.15028E-27	5.82777E-26	7.00359E-25	6.65626E-24	5.30884E-23	3.64450E-22	2.17874E-21	1.13336E-20	4.86701E-20
6	0.	4.71476E-25	8.62210E-24	1.02436E-22	9.62610E-22	7.59087E-21	5.15038E-20	3.04119E-19	1.56168E-18	6.62566E-18
7	0.	6.60990E-23	1.20011E-21	1.41674E-20	1.32354E-19	1.03762E-18	6.99635E-18	4.10227E-17	2.08951E-16	8.78057E-16
8	0.	8.43215E-21	1.51216E-19	1.76443E-18	1.63007E-17	1.26375E-16	8.42216E-16	4.87631E-15	2.45003E-14	1.01555E-13
9	0.	9.82735E-19	1.74948E-17	2.02988E-16	1.86651E-15	1.44057E-14	9.55315E-14	5.49750E-13	2.74052E-12	1.12497E-11
10	0.	1.00265E-16	1.76676E-15	2.03098E-14	1.85161E-13	1.41713E-12	9.31301E-12	5.30252E-11	2.60973E-10	1.05732E-09
11	0.	1.10824E-15	1.94933E-14	2.24062E-13	2.04512E-12	1.56793E-11	1.03168E-10	5.86927E-10	2.87584E-09	1.15500E-08
12	0.	1.19969E-14	2.09340E-13	2.39112E-12	2.17287E-11	1.66070E-10	1.08928E-09	6.16187E-09	2.98723E-08	1.18306E-07
13	0.	1.20168E-13	2.09457E-12	2.39989E-11	2.19617E-10	1.69560E-09	1.12482E-08	6.41467E-08	3.10692E-07	1.21666E-06
14	0.	1.08280E-12	1.87702E-11	2.15029E-10	1.97927E-09	1.54600E-08	1.04122E-07	6.00426E-07	2.89337E-06	1.10955E-05
15	0.	8.53620E-12	1.55507E-10	1.80708E-09	1.70568E-08	1.38156E-07	9.73304E-07	5.84836E-06	2.84369E-05	1.06337E-04
16	0.	6.44002E-11	1.12429E-09	1.33000E-08	1.29937E-07	1.11051E-06	8.41138E-06	5.43181E-05	2.65586E-04	9.41129E-04
17	0.	4.05015E-10	7.23012E-09	8.93715E-08	9.35621E-07	8.83458E-06	7.66245E-05	5.69812E-04	2.80519E-03	9.06228E-03
18	0.	2.01891E-09	3.71549E-08	4.89409E-07	5.63076E-06	6.10881E-05	6.52069E-04	6.00591E-03	2.89164E-02	7.85057E-02
19	0.	6.79918E-09	1.35920E-07	2.00235E-06	2.64526E-05	3.49972E-04	5.27381E-03	6.51463E-02	.31584	.61798
20	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

Table D-3.8

CALCULATED VALUES AT L = 1001. IT = 1

TIME = 9.1553E-03 SEC.

TEMPERATURE IN SOLID PHASE AT GRID POINT(MS,N)

N= MS	1	2	3	4	5	6	7	8	9	10
1	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0	3240.0
2	3143.6	3095.3	3093.4	3093.4	3093.4	3093.4	3093.4	3093.4	3093.4	3093.4
3	3047.3	2994.4	2992.3	2992.3	2992.2	2992.2	2992.2	2992.2	2992.2	2992.2
4	2952.4	2897.4	2895.2	2895.1	2895.1	2895.1	2895.1	2895.1	2895.1	2895.1
5	2857.4	2794.8	2792.1	2792.1	2792.0	2792.0	2792.0	2792.0	2792.0	2792.0
6	2763.0	2670.0	2665.8	2665.7	2665.7	2665.7	2665.7	2665.7	2665.7	2665.7
7	2669.0	2490.9	2484.1	2484.0	2483.9	2483.9	2483.9	2483.9	2483.9	2483.9
8	2399.7	2238.6	2232.5	2232.4	2232.4	2232.4	2232.4	2232.4	2232.4	2232.4
9	2114.3	1970.5	1964.8	1964.6	1964.6	1964.6	1964.6	1964.6	1964.6	1964.6
10	1842.9	1703.4	1697.8	1697.6	1697.6	1697.6	1697.6	1697.6	1697.6	1697.6
11	1575.2	1439.7	1434.3	1434.1	1434.1	1434.1	1434.1	1434.1	1434.1	1434.1
12	1311.1	1180.7	1175.5	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3	1175.3
13	1050.7	930.62	925.99	925.86	925.86	925.86	925.86	925.86	925.86	925.86
14	793.64	705.05	701.93	701.85	701.85	701.85	701.85	701.85	701.85	701.85
15	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00	540.00

NOTE
MS IS RADIAL GRID NUMBER IN SOLID PHASE
N IS GRID NUMBER IN AXIAL DIRECTION

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