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A THIN-SHOCK-LAYER SOLUTION
FOR NONEQUILIBRIUM, INVISCID
HYPERSONIC FLOWS IN EARTH,
MARTIAN, AND VENUSIAN ATMOSPHERES

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SUMMARY

An approximate inverse solution is presented for the nonequilibrium flow in the inviscid shock layer about a vehicle in hypersonic flight. The method is based upon a thin-shock-layer approximation and has the advantage of being applicable to both subsonic and supersonic regions of the shock layer. The relative simplicity of the method makes it ideally suited for programming on a digital computer with a significant reduction in storage capacity and computing time required by other more exact methods.

Comparison of nonequilibrium solutions for an air mixture obtained by the present method is made with solutions obtained by two other methods. Additional cases are presented for entry of spherical nose cones into representative Venusian and Martian atmospheres.

A digital computer program written in FORTRAN language is presented that permits an arbitrary gas mixture to be employed in the solution. The effects of vibration, dissociation, recombination, electronic excitation, and ionization are included in the program.

INTRODUCTION

The feasibility of planetary exploration has been the impetus for extensive research into problems associated with atmospheric entry of a blunted-nose vehicle. For the extreme velocities encountered, the gas flow in the shock layer about the vehicle can experience a severe departure from thermodynamic equilibrium. Analysis of the inviscid regime of the shock layer becomes rather complex and requires the simultaneous solution of the basic fluid-dynamic equations plus a system of coupled nonlinear equations governing the nonequilibrium rate processes. A further complication arises since the character of the system of fluid-dynamic partial differential equations changes from elliptic to hyperbolic as the flow changes from subsonic to supersonic.

Consequently, numerous techniques, each having its own peculiar advantages and disadvantages, have been used to investigate nonequilibrium blunt-body flows. The following techniques are discussed in reference 1: Newtonian approximations (refs. 2 and 3); streamtube method (refs. 4 to 6); inverse marching integration (refs. 7 to 10); integral relations (refs. 11 to 14); artificial viscosity and time asymptotic finite differences (refs. 15 and 16); series truncation (ref. 17); and boundary-layer-type approximations (refs. 18 to 20).

The present method is based upon the thin-shock-layer assumptions of Maslen (ref. 21). It requires specification of a shock shape and solves for the resultant body. This disadvantage is inherent in inverse methods, since, in general, the flow over a specified body is desired and the shock shape is not known. However, subsequent experience demonstrated that many desired body shapes could be obtained with some minor experimentation with the assumed shock shape. The analysis depends upon casting the governing flow equations in shock-oriented coordinates and then performing a Von Mises transformation so that the independent variables become the stream function and distance along the shock. An approximation is made to the momentum equation in the direction normal to the shock that enables it to be readily integrated. From this equation the pressure distribution in the Von Mises plane can be determined independently of the chemistry within the shock layer. The chemical and vibrational rate equations can then be integrated along streamlines. Transformation from the Von Mises plane to physical space is accomplished by numerical quadrature.

This approximate method of solution possesses three distinct advantages:

(1) Applicability throughout the subsonic and supersonic regions of an inviscid shock layer;

(2) Capability of handling a realistic model of an arbitrary gas mixture with a large number of chemical species and reactions in terms of reasonable computer memory storage; and

(3) Suitability for programing on a digital computer with significant reductions in computing times as compared with most existing methods.

Results obtained by use of this method for nonequilibrium air are compared with results from two other computational methods. Additional results are presented for entry of spherical nose cones into representative Venusian and Martian atmospheres.

This solution has been programed in FORTRAN IV and is presented with instructions for usage in appendix A by Barbara L. Weigel of the Langley Research Center. The program has the capability of handling up to 50 reactions and 25 species and includes the effects of vibrational relaxation, dissociation, vibration-dissociation coupling, electronic excitation, and ionization.

SYMBOLS

A	coefficient in equation (56)
A_j	frequency factor in rate constant for j th reaction
a	speed of sound, cm/sec
$a_{i,j}$	correlation integers for i th species in j th reaction (see appendix B)
B_j	temperature exponent in rate constant for j th reaction
c_i	mass fraction of i th species
E_j	activation energy in rate constant for j th reaction, K
e	internal energy per unit mass, ergs/g
$e_{e,i}$	electronic energy per unit mass of i th species, ergs/g
e_i	internal energy per unit mass of i th species, ergs/g
$e_{v,i}$	vibrational energy per unit mass of i th species, ergs/g
$\bar{e}_{v,i}$	equilibrium vibrational energy per unit mass of i th species, ergs/g
f_i	correlation factor: $f_i = 0$ for monatomic species; $f_i = 1$ for all other species
$g_{i,l}$	degeneracy of l th electronic energy level of i th species
ΔH_i	standard heat of formation at 0 K of i th species, ergs/mole
h	static enthalpy per unit mass, ergs/g
$\tilde{h} = h/V_\infty^2$	
K_j	rate constant for j th reaction, $(\text{moles})^{1-n}(\text{cm})^{3n-3}\text{sec}^{-1}$, where n is order of reaction

L_i	number of electronic energy levels for ith species
M	Mach number; general species in appendix B
M_f	$M_f = 0$, vibrational equilibrium; $M_f = 1$, vibrational nonequilibrium
m_j	code indicating which species to use when calculating coupling factor for jth reaction
N_i	number of vibrational energy levels included in dissociation energy of ith species
n	order of reaction
p	pressure, dynes/cm ²
$\tilde{p} = p/\rho_\infty V_\infty^2$	
q_k	general parameter representing either vibrational energy per unit mass or mass fraction of kth species
R	universal gas constant, 8.3147×10^7 ergs/mole-K
R_c	shock radius of curvature, cm
R_j	rate of reaction j per unit mass of mixture
$R_{j,j+1}$	ratio of forward rate to reverse rate of reaction j per unit mass of mixture
R_n	nose radius of body, cm
r	perpendicular distance from symmetry axis, cm
$\tilde{r} = r/R_N$	
$[S_i]$	moles per unit volume of ith species, moles/cm ³
S_J	$S_J = 1$ if $\nu_{I+1,j} = 0$; $S_J = \frac{a_{i,j}C_i}{\mu_i}$ if $\nu_{I+1,j} = 1$

T	temperature, K
$\tilde{T} = T/T_\infty$	
$T_{v,i}$	vibrational temperature of i th species, K
t	time, sec
u	velocity component in x-direction, cm/sec
V	velocity, cm/sec
v	velocity component in y-direction, cm/sec
x	distance along shock, cm
$\tilde{x} = x/R_n$	
y	distance normal to shock, cm
$\tilde{y} = y/y_b$	
z	distance along symmetry axis, cm
$\tilde{z} = z/R_n$	
$\alpha_{i,k}$	coefficient in vibrational relaxation time expression
$\beta_{i,k}$	temperature exponent in vibrational relaxation time expression
Δ_i	dissociation energy of i th species, K
δ	function defined in equation (49)
$\epsilon_{i,l}$	energy of l th electronic level of i th species, K
Θ_i	characteristic vibrational temperature, K
θ	local shock inclination angle (see fig. 1)

Λ	function defined in equation (47)
λ	scale factor $(1 - y)/R_c$
μ	molecular weight of gas mixture, g/mole
μ_i	molecular weight of ith species, g/mole
$\nu_{i,j}$	stoichiometric coefficient of ith reactant in jth reaction
$\nu'_{i,j}$	stoichiometric coefficient of ith product in jth reaction
$\nu_{I+1,j}$	stoichiometric coefficient of general species (see appendix B) in jth reaction
ρ	mass density, g/cm ³
$\tilde{\rho} = \rho/\rho_\infty$	
$\sigma_{i,k}$	coefficient in vibrational relaxation time expression
$\tau_{i,k}$	vibrational relaxation time of ith species due to vibrational energy exchange with kth species, sec
ϕ	angular position coordinate (fig. 1)
ϕ_j	coupling factor defined in equation (40)
ψ	stream function, g/sec
Ω	function defined in equation (48)
ω_k	general parameter in rate equation representing either the rate of production or rate of change of vibrational energy of species k

Subscripts:

b	body
s	shock

∞	free stream
0	behind shock on symmetry axis

ANALYSIS

Governing Equations

The solution described herein is an inverse method designed to take advantage of the characteristically thin shock layer that forms about a smooth axisymmetric body in hypersonic flight. If the shock-oriented coordinate system shown in figure 1 is adopted, the steady flow of an adiabatic, inviscid gas subject to nonequilibrium rate processes is governed by the following equations:

Continuity equation:

$$\frac{\partial}{\partial x}(\rho u r) + \frac{\partial}{\partial y}(\rho v \lambda r) = 0 \quad (1)$$

Momentum equations:

$$u \frac{\partial u}{\partial x} + \lambda v \frac{\partial u}{\partial y} - \frac{uv}{R_c} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0 \quad (2)$$

$$u \frac{\partial v}{\partial x} + \lambda v \frac{\partial v}{\partial y} + \frac{u^2}{R_c} + \frac{\lambda}{\rho} \frac{\partial p}{\partial y} = 0 \quad (3)$$

Energy equation:

$$h + \frac{u^2}{2} + \frac{v^2}{2} = \text{Constant} \quad (4)$$

Rate equation:

$$u \frac{\partial q_k}{\partial x} + \lambda v \frac{\partial q_k}{\partial y} = \lambda \omega_k(p, \rho, q_1, \dots, q_N) \quad (5)$$

Equation of state:

$$h = h(p, \rho, q_1, \dots, q_N) \quad (6)$$

In view of the thin shock layer, it is convenient to perform a Von Mises transformation. The stream function can be defined from the continuity equation by its partial derivatives,

$$\frac{\partial \psi}{\partial x} = \rho v r \lambda \quad (7)$$

and

$$\frac{\partial \psi}{\partial y} = -\rho u r \quad (8)$$

which leads to the transformation relationship

$$\left(\frac{\partial}{\partial x}\right)_{\psi} = \frac{\partial}{\partial x} + \frac{\lambda v}{u} \frac{\partial}{\partial y} \quad (9)$$

The resulting expressions for the momentum and rate equations are

$$\left(\frac{\partial u}{\partial x}\right)_{\psi} - \frac{v}{R_c} + \frac{\lambda v r}{u} \left(\frac{\partial p}{\partial \psi}\right)_x + \frac{1}{\rho u} \left(\frac{\partial p}{\partial x}\right)_{\psi} = 0 \quad (10)$$

$$\left(\frac{\partial v}{\partial x}\right)_{\psi} + \frac{u}{R_c} - \lambda r \left(\frac{\partial p}{\partial \psi}\right)_x = 0 \quad (11)$$

$$\left(\frac{\partial q_k}{\partial x}\right)_{\psi} = \frac{\lambda \omega_k}{u} \quad (12)$$

A differential form of the energy equation results from differentiating equation (4) and combining it with equations (2) and (3)

$$\left(\frac{\partial h}{\partial x}\right)_{\psi} = \frac{1}{\rho} \left(\frac{\partial p}{\partial x}\right)_{\psi} \quad (13)$$

The concept of a thin shock layer now makes certain simplifying approximations feasible. The flow within the inviscid shock layer is nearly parallel to the shock itself, except near the stagnation point. The term $\left(\frac{\partial v}{\partial x}\right)_{\psi}$ was neglected and the assumption was made that $\lambda \approx 1$. To this order of approximation, equations (11) and (12) become

$$\left(\frac{\partial p}{\partial \psi}\right)_x = \frac{u}{R_c r} \quad (14)$$

$$\left(\frac{\partial q_k}{\partial x}\right)_{\psi} = \frac{\omega_k}{u} \quad (15)$$

Adopting the approximation of Maslen (ref. 21), by using the values of r and u immediately behind the shock, allows equation (14) to be integrated along a normal to the shock and results in

$$p(x, \psi) = p_s(x) + \frac{u_s(x)}{R_c(x) r_s(x)} [\psi - \psi_s(x)] \quad (16)$$

At the shock

$$\psi_s = \frac{\rho_\infty V_\infty r_s^2}{2} \quad (17)$$

and on the body the boundary condition is

$$\psi_b = 0 \quad (18)$$

The effect of the approximations is to uncouple equation (11) from the remaining equations so that the resulting expression for the pressure (eq. (16)) is independent of the shock-layer chemistry and is a function only of the geometry and chemistry of the shock itself.

From the requirement of constant energy,

$$h + \frac{u^2}{2} + \frac{v^2}{2} = h_0 + \frac{v_0^2}{2} \quad (19)$$

Since the flow is nearly parallel to the shock, the approximation

$$v^2 - v_0^2 \ll u^2 \quad (20)$$

is made, and the following expression for the velocity u results:

$$u = [2(h_0 - h)]^{1/2} \quad (21)$$

In summary, equations (6), (13), (15), (16), and (21) form a determinate system of equations that can be integrated stepwise along streamlines to yield p , ρ , h , u , and q_k in the Von Mises plane. In addition to the boundary conditions of equations (17) and (18), the oblique shock relations (ref. 22) must be satisfied.

By noting the geometry of figure 1, the transformation back into physical (x,y) space can be accomplished by integrating equation (8) at constant x . The resulting expression

$$r = \left(r_s^2 - 2 \cos \theta \int_{\psi}^{\psi_s} \frac{d\psi}{\rho u} \right)^{1/2} \quad (22)$$

can be readily evaluated numerically.

The most important implication of the preceding analysis is that the equations are now applicable uniformly from the subsonic region through the supersonic region, except along the symmetry axis where the transformation is not well behaved.

Thermodynamic Model for a Reacting Gas

The gas under consideration is assumed to be a mixture of ideal gases. (See ref. 23.) The internal energy of the gas includes contributions from translation, rotation, vibration, dissociation, electronic excitation, and ionization.

The thermal equation of state is given by

$$p = \rho \frac{RT}{\mu} \quad (23)$$

with the mixture molecular weight given by

$$\mu = \left(\sum_{i=1}^I \frac{c_i}{\mu_i} \right)^{-1} \quad (24)$$

The mass fraction c_i is subject to the constraint

$$\sum_{i=1}^I c_i = 1 \quad (25)$$

The internal energy of the i th species can be expressed as

$$e_i = \frac{3}{2} \frac{RT}{\mu_i} + f_i \frac{RT}{\mu_i} + e_{v,i} + \frac{R}{\mu_i} \frac{\sum_{l=1}^{L_i} g_{i,l} \epsilon_{i,l} \exp\left(\frac{-\epsilon_{i,l}}{T}\right)}{\sum_{l=1}^{L_i} g_{i,l} \exp\left(\frac{-\epsilon_{i,l}}{T}\right)} + \frac{\Delta H_i}{\mu_i} \quad (26)$$

where the rotational (rigid rotor) and electronic energy modes are assumed to be in equilibrium with the translational mode. In the computer program to be described subsequently, two options exist for computing the vibrational (linear harmonic oscillator) energy. In the first option, the vibrational mode is assumed to be in equilibrium with the translational mode and $e_{v,i}$ is calculated from

$$e_{v,i} = \frac{f_i R \Theta_i}{\mu_i \left[\exp\left(\frac{\Theta_i}{T}\right) - 1 \right]} \quad (27)$$

The second option is for vibrational nonequilibrium and $e_{v,i}$ is determined by integration of the vibrational rate equation along a streamline.

Since a mixture of ideal gases has been assumed, the total energy is

$$e = \sum_{i=1}^I c_i e_i \quad (28)$$

The enthalpy is defined as

$$h = e + \frac{p}{\rho} \quad (29)$$

By referring to the previous equations, it can be seen that

$$h = h(p; \rho; e_{v,i}, \dots, e_{v,I}; c_i, \dots, c_I) \quad (30)$$

which agrees with the form stated in equation (6).

Rate Equations

The general rate expression given in equation (5) must be specialized for chemical processes and for vibrational relaxation. The resultant equation must be capable of describing a system of chemical species ($i = 1, 2, 3, \dots, I$) and the associated kinetic reactions ($j = 1, 2, 3, \dots, J$).

Chemical processes.— An arbitrary one-step chemical reaction can be described by



The law of mass action (ref. 23) requires the rate of production of a species to be proportional to the product of the concentrations of the reacting species, each concentration being raised to a power equal to its stoichiometric coefficient. The net rate of production of S_i per unit mass of mixture is then

$$\frac{d\left(\frac{[S_i]}{\rho}\right)}{dt} = \frac{K}{\rho} (\nu'_i - \nu_i) \prod_{i=1}^I [S_i]^{\nu_i} \quad (32)$$

Since

$$[S_i] = \frac{\rho c_i}{\mu_i} \quad (33)$$

equation (32) can be generalized for a system of J simultaneous reactions and put in the form of equation (12). As a result,

$$\left[\left(\frac{\partial c_i}{\partial x} \right)_{\psi} \right]_j = \frac{K_j \mu_i}{\rho u} (\nu'_{i,j} - \nu_{i,j}) \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i} \right)^{\nu_{i,j}} \quad (34)$$

The total rate of production is

$$\left(\frac{\partial c_i}{\partial x}\right)_\psi = \sum_{j=1}^J \left[\left(\frac{\partial c_i}{\partial x}\right)_\psi\right]_j \quad (35)$$

The specific reaction rate constant is given by

$$K_j = A_j T^{B_j} \exp\left(\frac{-E_j}{T}\right) \quad (36)$$

Equation (34) is applicable to opposing reactions if the forward and reverse reactions are treated separately.

If the rate constants for the reaction of a chemical species with several catalytic species are the same, provision can be made to incorporate all these catalysts into a single reaction by introducing a "general species." (See appendix B.) The resulting rate expression is now

$$\left[\left(\frac{\partial c_i}{\partial x}\right)_\psi\right]_j = \left[\frac{K_j \mu_i}{\rho u} (\nu'_{i,j} - \nu_{i,j}) \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i}\right)^{\nu_{i,j}}\right] \left[\rho \sum_{i=1}^I \frac{c_i a_{i,j}}{\mu_i}\right]^{\nu_{I+1,j}} \quad (37)$$

Vibrational relaxation.- If the vibrational rate equation developed in reference 24 for a multicomponent gas mixture is written in the form of equation (12), the result is

$$\left(\frac{\partial e_{v,i}}{\partial x}\right)_\psi = \frac{1}{u} \sum_{k=1}^I \frac{c_k}{\tau_{i,k}} (\bar{e}_{v,i} - e_{v,i}) \quad (38)$$

where $\bar{e}_{v,i}$ is the equilibrium vibrational energy from equation (27) and $e_{v,i}$ is the vibrational energy. The relaxation time $\tau_{i,k}$ can be expressed as

$$\tau_{i,k} = \frac{\alpha_{i,k} T^{\beta_{i,k}} \exp(\sigma_{i,k} T^{-1/3})}{p \left[1 - \exp\left(\frac{-\Theta_i}{T}\right)\right]} \quad (39)$$

which is of the form predicted by classical Landau-Teller theory. Although equations (38) and (39) were formulated on the assumption of a system of harmonic oscillators having a single vibrational mode, polyatomic molecules with several vibrational modes can be handled in the computer program if it is assumed that they are independent of one another

and the relaxation frequencies for the individual modes are combined into a single equivalent frequency. (See ref. 23.)

Coupling of vibrational relaxation and dissociation.- It has been pointed out in the literature (for example, refs. 25 to 28) that the processes of vibrational relaxation and dissociation do not occur independently, but rather each process influences the other. The CVD (coupled-vibration-dissociation) model of Hammerling et al. (ref. 25) was chosen for this analysis. Without discussing the relative merits of the various other coupling models, it should be noted that another model could be incorporated into this method with little difficulty.

Since molecules with vibrational energy less than that corresponding to equilibrium with the translational energy do not dissociate as readily as predicted by the dissociation rate constant for vibrational equilibrium, the CVD model develops a correction to the rate constant. From reference 25 the coupling coefficient is

$$\phi_j = \frac{1}{N_i} \left\{ \frac{1 - \exp \left[-N_i \left(\frac{\Theta_i}{T_{v,i}} - \frac{\Theta_i}{T} \right) \right]}{\exp \left(\frac{\Theta_i}{T_{v,i}} - \frac{\Theta_i}{T} \right) - 1} \right\} \left[\frac{\exp \left(\frac{\Theta_i}{T_{v,i}} \right) - 1}{\exp \left(\frac{\Theta_i}{T} \right) - 1} \right] \quad (40)$$

The number of vibrational states N_i is the smallest integer so that

$$N_i > \frac{\Delta_i}{\Theta_i} \quad (41)$$

Inserting the coupling coefficient in equation (37) results in

$$\left[\left(\frac{\partial c_i}{\partial x} \right)_{\psi_j} \right] = \left[\frac{\phi_j K_j \mu_i}{\rho u} (\nu'_{i,j} - \nu_{i,j}) \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i} \right)^{\nu_{i,j}} \right] \left[\rho \sum_{i=1}^I \frac{c_i a_{i,j}}{\mu_i} \right]^{\nu_{I+1,j}} \quad (42)$$

For a dissociation reaction, ϕ_j can be calculated from equation (40); for other reactions, ϕ_j is unity.

SOLUTION PROCEDURE

Initial Conditions

An inverse method presupposes specification of the shock shape. In all cases described herein, an analytical expression of the form

$$r_s = r_s(z) \quad (43)$$

was used. From this relationship, θ , R_c , and x can be given by

$$\theta = \arctan\left(\frac{dr_s}{dz}\right) \quad (44)$$

$$R_c = \frac{\left[1 + \left(\frac{dr_s}{dz}\right)^2\right]^{3/2}}{\left|\frac{d^2r_s}{dz^2}\right|} \quad (45)$$

and

$$x = \int_0^{r_s} \frac{dr_s}{\sin \theta} \quad (46)$$

After determining the shock parameters, initiation of the solution begins with calculation of free-stream conditions. With selected values of p_∞ , T_∞ , V_∞ , and a specified gas composition, equations (23) to (28) can be utilized to calculate μ_∞ , ρ_∞ , and e_∞ .

The next step requires determining the state of the gas immediately behind the shock wave. The shock wave is assumed to be a discontinuity, translational, rotational, and electronic contributions to the internal energy of the gas reaching instantaneous equilibrium at the translational temperature behind the shock T_s . The vibrational energy may be treated as being in equilibrium with the other energy modes or optionally it may be described by a system of harmonic oscillators with a Boltzmann distribution about a nonequilibrium vibrational temperature. Species concentrations are assumed to be frozen through the shock.

An iterative procedure is required to solve the oblique-shock-conservation relations. From the shock geometry and the free-stream conditions, the following parameters can be calculated:

$$\Lambda(x) = \rho_\infty V_\infty \sin \theta \quad (47)$$

$$\Omega(x) = p_\infty + \rho_\infty V_\infty^2 \sin^2 \theta \quad (48)$$

$$\delta(x) = e_\infty + \frac{p_\infty}{\rho_\infty} + \frac{V_\infty^2 \sin^2 \theta}{2} \quad (49)$$

With an initial estimate of T_s , the energy e_s can be determined from equations (26) to (28). The temperature and energy are further related by

$$T_S = \frac{2\mu_\infty(\delta - e_S)\sqrt{\Omega^2 - 2\Lambda^2(\delta - e_S)}}{R\left[\Omega + \sqrt{\Omega^2 - 2\Lambda^2(\delta - e_S)}\right]} \quad (50)$$

Equation (50) can be iterated until subsequent values of T_S differ by a sufficiently small amount. After convergence

$$p_S = \sqrt{\Omega^2 - 2\Lambda^2(\delta - e_S)} \quad (51)$$

$$\rho_S = \frac{p_S \mu_\infty}{RT_S} \quad (52)$$

$$h_S = e_S + \frac{p_S}{\rho_S} \quad (53)$$

$$u_S = V_\infty \cos \theta \quad (54)$$

The pressure distribution in the x, ψ plane can now be calculated from equation (16).

Integration Method

Since the initial conditions and the pressure distribution have been determined, equations (13), (37), and (38) can be integrated stepwise along streamlines. It was found that for the cases investigated herein, the system of equations exhibited the so-called "stiff" behavior. (See refs. 29 and 30.) The integration scheme proposed by Treanor (ref. 31) was chosen for its ability to handle the stiff equations with significant reductions in computational times compared with both the fourth-order Runge-Kutta method (ref. 32) and the Adams-Moulton method using the fourth-order Runge-Kutta method for starting (ref. 33).

A special problem occurs for the $\psi = 0$ or body streamline. On all other streamlines the integration begins immediately behind the shock and proceeds from there. However, on the Z-axis the transformation of the governing equations is ill-behaved since x and ψ are both zero. Therefore, the integration cannot proceed from behind the shock along the stagnation streamline with the equations in their present form.

The $\psi = 0$ streamline integration was accomplished in the following manner. The initial interval Δx on the shock wave was divided into five subintervals. The rate equations were integrated from behind the shock at each subinterval to the point $x = \Delta x$. The values of the variables as a function of ψ were then extrapolated along $x = \Delta x$ to the

body ($\psi = 0$). Integration along the $\psi = 0$ streamline can proceed from there. Five subintervals were decided to be adequate after experimenting with up to 15 subintervals.

Transformation to Physical Space

Upon completion of the integration along streamlines, the thermodynamic properties, the velocity u , and the species concentrations are known functions of x and ψ . Equation (22) can then be evaluated numerically by Simpson's rule to obtain r . Evaluation of the flow field is thus completed.

RESULTS AND DISCUSSION

In order to investigate the capabilities of the present method of solution, cases have been computed for numerous shock shapes and gas mixtures. A number of representative cases have been selected for presentation. Case I is a comparison of results for nonequilibrium air with the more exact inverse method of reference 8. Case II is a comparison of the results for nonequilibrium air with the streamtube method used in reference 34. Cases III, IV, and V present results for entry of spherical nose cones into representative Martian and Venusian atmospheres.

Case I

This example was computed to compare with the results of reference 8 for a catenary shock ($R_{c,0} = 2.11$ cm) with a free-stream velocity of 7.01×10^5 cm/sec at 61 km. The reactions and rates given in appendix C are the same as those used in reference 8. Vibrational equilibrium was assumed.

Figure 2 indicates excellent agreement with the results of reference 8 for the body shape and the location of a streamline crossing the shock at an angle θ of 81° ($x/R_{c,0} = 0.16$). The variations of the temperature, pressure, density, and species mole fractions along this streamline are compared with the corresponding results from reference 8 in figures 3, 4, 5, and 6, respectively. As should be expected, the effect of neglecting the velocity gradient term in equation (11) is to predict the pressure to be lower than the actual value at a given x . This effect can be expected to diminish as the flow proceeds away from the stagnation region and becomes more nearly parallel to the shock.

Initially, the flow along this streamline exhibits behavior similar to that behind a normal-shock wave with density increasing with sharply falling temperature. However, as the flow expands away from the nose, the density reaches a maximum and begins to decrease as the temperature continues to decrease.

Concentrations of N, O, NO, and e^- shown in figure 6 indicate very good agreement with the results of reference 8. The greatest error occurs for NO shown in figure 6(c), the present method predicting the concentrations about 20 percent too high at worst.

Variations of the pressure, temperature, density, and species concentrations across the shock layer at $\theta = 81^\circ$ are shown in figures 7, 8, 9, and 10, respectively. Again, the agreement with the results of reference 8 is good. From this comparison it may be concluded that the present method gives good agreement with the exact method near the stagnation region which represents a severe test of the approximations inherent in the present method.

Case II

This example was selected for comparison with the nonequilibrium air results of reference 34 for flow over a 9° half-angle cone with a spherical nose (30.48-cm diameter) at an altitude of 47.5 km. The equation

$$r_s^2 = -0.3625z_s^2 + 36.064z_s - 0.1767r_s z_s \quad (55)$$

was fitted in the nose region to the shock points computed in reference 34. Although Evans, and others, used a sophisticated system of 13 species and 54 reactions, the approximate air model used in case I was used for this comparison. Vibrational nonequilibrium was assumed.

It can be seen in figure 11 that the present method predicts the body shape extremely well. A comparison of the surface pressures and temperatures as calculated by both methods is presented in figures 12 and 13, respectively. In general, the agreement is seen to be good. There is a discrepancy in the temperature calculations close to the symmetry axis, but this condition improves rapidly with increasing distance. Both methods are admittedly inaccurate in the region where the discrepancy occurs. Finally, the electron concentration on the body surface is shown in figure 14. The prediction of the present method is understandably lower since the reaction scheme permits only the NO^+ ion. Agreement improves further back on the surface. This result might be expected since figure 7 of reference 34 indicates NO^+ is the major ion present after the flow expands past the sphere-cone tangency point.

Case III

This case was computed for ballistic entry into a Venusian atmosphere. It was found that shock shapes of the form given by

$$z_s = \frac{r_s^2}{1 + Ar_s} \quad (56)$$

would generate bodies that approximate part of a sphere-cone. The parameter A represents the slope of the asymptote of the shock for large values of r_s . For sufficiently large apex angles under appropriate conditions, the flow over the face of a truncated sphere-cone is subsonic, the sonic point being on the body at the sharp corner where the transition to supersonic flow occurs. There is a resultant rapid drop in pressure near the corner. It should be noted that a shock shape of the form of equation (56) can be used to calculate the flow in the shock layer up to the point where the rapid pressure drop occurs, but another equation would be required for the shock where it "bends" as the flow expands around the sonic corner. However, in this rapidly expanding flow region, the approximations inherent in this method of analysis would not be valid.

According to recently available information on Venus (ref. 35), the atmosphere is almost entirely carbon dioxide. Therefore, a 100-percent CO_2 mixture was assumed and the kinetic reactions and rates shown in appendix C were used. Vibrational nonequilibrium was assumed. The free-stream conditions are

$$V_\infty = 8.69 \times 10^5 \text{ cm/sec}$$

$$\rho_\infty = 1.4175 \times 10^{-6} \text{ g/cm}^3$$

$$T_\infty = 200 \text{ K}$$

The assumed shock ($A = 1.732$) and the computed body which approximates a 57° half-angle sphere-cone are shown in figure 15. Pressure, density, and temperature variations along streamlines crossing the shock at $\tilde{x} = 0.5$ and 2.0 are presented in figures 16, 17, and 18, respectively. Figure 16 indicates that the pressure along both streamlines approaches the same constant level as the flow progresses away from the shock as would be expected for cone flow.

Species concentrations along these streamlines are shown in figure 19. Figure 19(a) indicates that the CO_2 disappears rapidly with increasing distance while the C and O concentrations increase along the inner streamline ($\tilde{x} = 0.5$). The CO concentration increases to a maximum and then decreases. Figure 19(b) shows similar behavior along the outer streamline ($\tilde{x} = 2.0$). This behavior is the same as that observed by Howe, Viegas, and Sheaffer (ref. 36) behind normal shocks in CO_2 at slightly different ambient conditions. Their gas model however did not include the effects of vibrational relaxation or ionization. Figure 19(c) indicates that the concentrations of the electrons and the C^+ and O^+ ions increase with distance whereas CO^+ reaches a maximum and then begins to decrease along the inner streamline ($\tilde{x} = 0.5$). The same behavior is exhibited along the outer streamline ($\tilde{x} = 2.0$) except that the CO^+ has not reached a maximum and begun to decrease, as shown in figure 19(d). Along both streamlines, the dominant electron-producing reaction is the

ionization of CO. The C_2 concentrations shown in figures 19(e) and 19(f) are several decades lower than the concentrations of the other species.

The pressure and temperature distributions along the surface of the body are shown in figures 20 and 21, respectively. Figure 22 presents species concentrations along the body surface. On the body surface the longer particle residence times have allowed more CO dissociation and resulted in most of the electrons being formed from ionization of C and O. This result is in contrast to the results shown along the inner and outer streamlines.

Figure 23 is a profile of the static enthalpy across the shock layer at $\tilde{x} = 2.0$. It can be seen that the enthalpy increases sharply near the body. This region near the body is known as the entropy layer. Gas particles in this region have experienced a much larger rise in entropy from traversing the shock closer to the stagnation streamline and, as a result, much of the kinetic energy was converted to thermal energy. Pressure and temperature profiles across the shock layer at $\tilde{x} = 2.0$ are shown in figure 24. A typical electron concentration profile across the shock layer is shown in figure 25. It can be seen that the concentration builds up rapidly within the entropy layer near the body.

Case IV

This example was selected to represent entry into a possible Martian atmosphere having a composition of 95 percent CO_2 and 5 percent A by mass. The free-stream conditions are:

$$V_{\infty} = 4.572 \times 10^5 \text{ cm/sec}$$

$$\rho_{\infty} = 1.068 \times 10^{-5} \text{ g/cm}^3$$

$$T_{\infty} = 200 \text{ K}$$

The scheme of kinetic reactions and rates used in this example is given in appendix C. Vibrational nonequilibrium was assumed. After some experimentation it was found that a shock shape of the form

$$z_s = \frac{r_s^2}{1 + 1.89r_s} \quad (57)$$

resulted in the body shown in figure 26 which closely approximates a 60° half-angle sphere-cone with a 1-cm nose radius. Pressure and temperature variations along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6 are shown in figures 27 and 28.

Species concentrations along these same streamlines are presented in figure 29. The CO_2 concentration decreases rapidly with increasing distance as it dissociates into

CO and O and results in the increasing concentrations of these species shown in figure 29(a). It is seen from figure 29(c) that the dominant ion present is CO^+ .

Figure 30 illustrates the pressure and temperature variations along the surface of the body. Species concentrations along the body are presented in figure 31. It can be seen that the peak electron concentration on the surface occurs near the nose. The electrons are seen to result primarily from ionization of CO as was the case on the streamlines within the shock layer.

The sudden rise in static enthalpy within the entropy layer is shown in figure 32 for $\tilde{x} = 1.6$. Pressure and temperature profiles across the shock layer at this value of $\tilde{x}$ are shown in figure 33. Figure 34 illustrates the variation in the electron concentration across the shock layer. A marked increase in electron concentration is observed within the entropy layer.

Investigation of the assumed reaction mechanism for this case indicates that the chemical kinetics are controlled predominantly by two-body collision processes. Since the three-body recombination reactions are relatively unimportant, the remainder of the reactions are two-body collisions having the same density dependence. For specified initial temperature and species concentrations, the time (or distance) variation of all variables can then be scaled with respect to density. Practically, this concept of binary scaling (ref. 8) means that for a given flight velocity, flows will be similar if the product of ambient density and nose radius is held constant. For this particular case the results would then apply for a body with nose radius of 30.48 cm and $\rho_\infty = 3.5 \times 10^{-7} \text{ g/cm}^3$. These conditions might be typical of a Viking-type entry on Mars.

To demonstrate the validity of the binary scaling assumption, it is necessary to assess the importance of three-body recombination reactions for this system. Define the rate of reaction j per unit mass of mixture as

$$R_j = \left[\frac{K_j}{\rho} \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i} \right)^{\nu_{i,j}} \right] \left(\rho \sum_{i=1}^I \frac{c_i a_{i,j}}{\mu_i} \right)^{\nu_{I+1,j}} \quad (58)$$

and define the ratio

$$R_{j,j+1} = R_j / R_{j+1} \quad (59)$$

The ratio $R_{j,j+1}$ can then be used to judge the relative importance of the forward rate to the reverse rate of a reaction.

Shown in figure 35 are the ratios along the inner streamline ($\tilde{x} = 0.4$) of the forward rate for the system of reactions as numbered in appendix C for this case. It can be seen

that $R_{j,j+1} \gg 1$ for all the reactions involving three-body recombinations except $R_{3,4}$ which indicates that the recombination of C and O to form CO is becoming more important far from the shock on this streamline. However, at the furthestmost point, $R_{3,4} \approx 6$; therefore, the assumption that the flow along this streamline can be scaled is probably still a reasonable approximation. A true test of the validity of binary scaling in this case would require repeating the calculation for various values of ρ_∞ for constant $\rho_\infty R_n$ and comparing the results.

Case V

This example is similar to Case IV with the same free-stream conditions and kinetic reactions, but with a composition of 50 percent CO_2 and 50 percent A by mass. After some experimentation it was found that the shock shape given by

$$z_s = \frac{r_s^2}{1 + 1.98r_s} \quad (60)$$

results in the body shown in figure 36 which closely approximates a 60° half-angle sphere-cone with a 1-cm nose radius. The shock standoff distance is greater for this case than that for Case IV because of the lower density ratio across the shock for this mixture. Pressure and temperature variations along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6 are shown in figures 37 and 38. Comparing figures 28 and 38 shows that the temperature in the shock layer is about 10 percent higher for this case. The variations of species concentrations along these streamlines are presented in figure 39. Comparison with figure 29 from Case IV shows essentially the same behavior. Again, the predominant ion is CO^+ . The electron concentrations are somewhat higher for this case because of the higher temperature in the shock layer.

Pressure and temperature variations on the body surface are shown in figure 40. Figure 41 illustrates variations of species concentrations on the surface. The only obvious difference in the profiles from those of Case IV appears in the electron concentration. In the previous case the profile reached a maximum near the sphere-cone juncture and then decreased. For this case the profile decreases monotonically with increasing distance.

Existence of the entropy layer is again demonstrated by the rapid increase in static enthalpy near the surface shown in figure 42 for $\tilde{x} = 1.6$. Pressure and temperature distributions across the shock layer at this value of $\tilde{x}$ are shown in figure 43. The variation in electron concentration across the shock layer at this value of $\tilde{x}$ is shown in figure 44 to be about a factor of 10 higher than that for Case IV.

The ratio of forward reaction rates to reverse reaction rates for this reaction system as given in appendix C is shown in figure 45. It can be seen that all $R_{j,j+1} \gg 1$ for

the three body recombination reactions. Thus, the binary-scaling assumption appears to be justifiable for this case.

CONCLUDING REMARKS

An approximate inverse solution is presented for the nonequilibrium flow in the inviscid shock layer about a vehicle in hypersonic flight. A number of representative cases have been presented. Case I is a comparison of results for nonequilibrium air with the more exact inverse method. Case II is a comparison of the results for nonequilibrium air with the streamtube method. Cases III, IV, and V present results for entry of spherical nose cones into representative Martian and Venusian atmospheres. From the foregoing analysis and results, the following observations can be made.

The method of solution as programed herein can handle a realistic model of an arbitrary gas mixture with large numbers of chemical reactions and species. A larger number of reactions and/or species could be easily accommodated by increasing the dimensioning of the appropriate variables in the FORTRAN program. The gas model permits consideration of vibrational relaxation, dissociation, recombination, ionization, electronic excitation, and vibration-dissociation coupling. With relative ease the gas model could be made more sophisticated. For example, the vibrational partition function could include effects of anharmonicity or a more realistic vibration-dissociation coupling model could be included.

Many flow-field solutions suffer the disadvantage of being valid only in the subsonic (or supersonic) region of a shock layer. Another method is required to solve the supersonic (or subsonic) region so that the solutions match in the transonic zone. The approximations inherent in the method presented herein avoid this difficulty and render the method applicable for subsonic and supersonic flows.

The solution offers little difficulty in programing for use on a digital computer as evidenced by the program described herein. Primarily because of the approximations made to the governing equations, this method offers the possibility of significant reductions in computing time. The required computing time for Case I on the Control Data 6600 digital computer was 79 seconds. The remaining 4 cases required between 5 and 14 minutes of time, Case II requiring the maximum time. These times are based upon calculating 20 streamlines. This result appears to be a significant reduction in the times reported in most of the existing literature on nonequilibrium flow fields.

The accuracy of the present method compared extremely well with the inverse marching integration technique for Case I and the streamtube method for Case II. Although the method fails on the Z-axis and the approximations are crude close to the

stagnation point, the requirements of a thin shock layer and a smooth symmetric body are not so restrictive that application of the method is unduly hindered.

For Case III the electron concentrations were found to be greatest near the body in the entropy layer. In this region the electrons are produced primarily from ionization of C and O atoms. Within the shock layer, but outside the entropy layer, the concentrations are lower and the major ion present is CO^+ .

For Case IV the electron concentrations were found to be greatest in the entropy layer. Throughout the shock layer the major ion present is CO^+ . Maximum electron concentration occurred near the nose on the body.

The assumption of binary scaling for this system of reactions used in this case appeared to be a justifiable approximation. It was evident, however, that the recombination of C and O to form CO is the critical reaction in determining the validity of this assumption.

The larger percentage of argon for Case V compared with Case IV results in the argon acting as a nondissociating diluent with resulting higher temperatures in the shock layer. The electron concentrations are correspondingly higher. Maximum concentrations exist in the entropy layer. The binary-scaling assumption again appears to be justifiable for case V.

It should be emphasized that the systems of reactions chosen for these cases are merely representative and by no means definitive. Possible inaccuracies may arise if an incomplete reaction mechanism is used.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., October 28, 1971.

APPENDIX A

A COMPUTER PROGRAM TO DETERMINE THE FLOW FIELD IN A NONEQUILIBRIUM SHOCK LAYER ABOUT A SMOOTH SYMMETRIC BODY TRAVELING AT HYPERSONIC SPEEDS USING AN INVERSE TECHNIQUE

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Introduction

This appendix describes the digital computer program (LRC Program D1290) developed to support the study of an inverse technique (shock-shape specified) for determining the flow field in a nonequilibrium shock layer about a smooth symmetric body traveling at hypersonic speeds. The problem description, development of governing equations, symbols, method of solution, and results are discussed in the text of this paper.

Problem Description

The problem of determining the flow field in a shock layer about a smooth symmetric body behind a specified shock shape may be divided into six parts:

- (1) Computation of the shock geometry (x_s , z_s , r_s , R_c , $\cos \theta$, and $\sin \theta$) from a definition supplied by the user. (See fig. 1)
- (2) Computation of the free-stream quantities (μ_∞ , ρ , a_∞ , M_∞ , and e_∞)
- (3) Computation of quantities immediately behind the shock (e_s , T_s , p_s , ρ_s , u_s , and ψ_s)
- (4) Computation of pressures, and their derivatives, in the flow field ($p(x, \psi)$ and $\frac{dp}{dx}(x, \psi)$)
- (5) Integration along streamlines from a point just behind the shock to a point sufficiently downstream to define the flow field
- (6) Computation of physical space quantities r , y , and z , at specified points in the flow field to give a good body and flow field definition

APPENDIX A - Continued

Numerical Methods

The numerical methods used for the development of this program include

- (1) A modified Runge-Kutta integration scheme designed for chemical problems (ref. 31)
- (2) The Newton-Raphson iteration method (ref. 37, p. 192)
- (3) Numerical differential equations (ref. 38, p. 96)
- (4) Simpson's Rule integration technique (ref. 39, p. 137)
- (5) Trapezoidal Rule integration technique (ref. 39, p. 142)

Subprograms

The subprograms used are given in the following listing:

FORTTRAN name	Called by	Function
SHOCKG	D1290	to compute the shock geometry and store on tape 10
FDPDX	D1290	to evaluate the pressure p and its derivative $\dot{p}$ and store on tapes
FOFTS	ITR1	to evaluate T_s
ITR1	BASIC	to iterate for e
ITR1	D1290	to iterate for T_s
CALINTH	D1290	to obtain the integration technique
BASIC	CALINTH	to evaluate the derivatives $\dot{h}$, $\dot{c}_i$, and $\dot{e}_{v,i}$ for $i = 1, I$
FOFE	ITR1	to evaluate e
CHECK	CALINTH	to test results of an integration step and accept or reject the results

APPENDIX A - Continued

Subprogram SHOCKG(DELX,ZSTERM,IZTERM) is called by D1290 to compute the shock geometry parameters and store them on tape 10. This subroutine must be supplied by the user to define the shock shape desired. The calling sequence must contain the two input quantities DELX and ZSTERM and a generated integer, IZTERM, the number of x values computed in the subroutine. The user must store the following parameters on tape 10: x , z , r , R_C , $\cos \theta$, and $\sin \theta$. These six parameters must be computed at each x from $x = 0$ to $x \geq ZSTERM$ and x must be in increments of DELX/5 to DELX and increments of DELX thereafter until $x \geq ZSTERM$ where

x	distance along shock, cm
z	distance along symmetry axis, cm
r	perpendicular distance from symmetry axis to shock, cm
R_C	radius of curvature of shock, cm
θ	local shock inclination angle, radians

STOP 13 has been used for error stops in this subroutine. In the sample case, the following shock shape was defined:

$$z = \cosh r - 1.0$$

$$x = \sqrt{2z + z^2}$$

$$\cos \theta = \frac{x}{\sqrt{x^2 + 1.0}}$$

$$R_C = 1.0 + x^2$$

Iteration of e

To encourage iteration to an acceptable value of e and thereby reduce instability, the following tests have been used:

(1) If the maximum number of iterations (10) is exceeded before convergence is reached, a new estimate of e is computed and the iteration is again attempted. The program will restart this iteration twice. If convergence is not reached, the program will terminate with STOP 66.

(2) If the converged e is greater than h and a negative T results, e is set equal to $h - 0.000001 * h$ and one more iteration on e is attempted.

APPENDIX A - Continued

(3) If, after this maneuver, e is again greater than h , a trigger is set to restart the integration interval at one-fourth the current computing interval.

Testing Results of Integration

After an integration interval has been computed, several tests are made to decide whether to

- (1) Continue,
- (2) Recompute at one-fourth the current computing interval, or
- (3) Stop the case.

Trial and error has proved that recomputing at a smaller interval sometimes prevents instabilities and error conditions from developing.

Stagnation Streamline

The stagnation $\psi = 0.0$ streamline is computed after the streamlines

$$\psi = \frac{\Delta x}{5}, \frac{2\Delta x}{5}, \frac{3\Delta x}{5}, \text{ and } \frac{4\Delta x}{5}$$

have been integrated to $x = \Delta x$. Values of e , T , h , c_i , and e_i ($i = 1, I$) at $\psi = 0.0$ are obtained by extrapolation. Then $T_{v,i}$ ($i = 1, I$), u , ρ , p , and $\dot{p}$ values are computed and the $\psi = 0.0$ streamline is integrated from Δx to $x \geq Z\text{TERM}$.

Negative u^2

In the evaluation of the derivatives if u^2 becomes negative, the integration is discontinued and an attempt is made to compute the physical space values for the calculated flow field.

Input

The data input is loaded by using FORTRAN IV NAMELIST. One card, 80 columns, is read in by FORMAT (8A10) for case identification. The input symbols are as follows:

FORTRAN name	Symbol	Description
\$NAM1		
DELX	Δx	increment along shock, cm
ZSTERM		length of symmetry axis, z , cm

APPENDIX A - Continued

FORTTRAN name	Symbol	Description
IMAX	I	maximum number of species i , ≤ 25
JMAX	J	maximum number of reactions j , ≤ 50
MJ	m_j	an array containing an integer indicating which species i to use to calculate the coupling factor ϕ_j for reaction j
M	M_f	1, vibrational nonequilibrium; 0, vibrational equilibrium
R	R	universal gas constant, ergs/mole-K
GAMMA	γ	ratio of frozen specific heats
CIINF	$c_{i,\infty}$	an array containing free-stream mass fraction for each species i
PINF	p_∞	free-stream pressure, dynes/cm ²
TINF	T_∞	free-stream temperature, K
VINF	V_∞	free-stream velocity, cm/sec
MUI	μ_i	an array containing molecular weight for each species i , g/mole
BJ	B_j	an array containing temperature exponent for each reaction j in Arrhenius-type rate equation
EJ	E_j	an array of activation energies for each reaction j , K
ALJ	$a_{i,j}$	a two-dimensional array of correlation factors for i th species in j th reaction

APPENDIX A - Continued

FORTTRAN name	Symbol	Description
NULJ	$\nu_{i,j}$	a two-dimensional array of stoichiometric coefficients of ith reactant in jth reaction
NUPLJ	$\nu'_{i,j}$	a two-dimensional array of stoichiometric coefficients for ith product in jth reaction
ALPIK	$\alpha_{i,k}$	a two-dimensional array of coefficients in vibrational relaxation time expression
BETAIK	$\beta_{i,k}$	a two-dimensional array of temperature exponents in vibrational relaxation time expression
SIGIK	$\sigma_{i,k}$	a two-dimensional array of coefficients in vibrational relaxation time expression
THETAI	Θ_i	an array containing characteristic vibrational temperature K for each species i
DGENI	g_i	an array of factors for each species i to permit approximating a polyatomic molecule by a diatomic molecule
FI	f_i	an array of correlation factors for each species i, 0.0 for monatomic species and 1.0 for all others
DELHI	ΔH_i	an array of standard heat of formation at 0 K for each species i, ergs/mole
DELI	Δ_i	an array of dissociation energy for each species i, K
EVI	$e_{v,i}$	an array of vibrational energy per unit mass for each species i, ergs/g

APPENDIX A – Continued

FORTTRAN name	Symbol	Description
LI	L_i	an array containing number of electronic levels for each species i
GIL	$g_{i,l}$	a two-dimensional array containing degeneracy of LI electronic levels for each species i
EPSIL	$\epsilon_{i,l}$	a two-dimensional array containing energy of LI electronic levels for each species i , °K
AJ	A_j	an array containing frequency factor, $\text{cm}^{3n}/\text{mole}^n\text{-sec}$, for each reaction j in Arrhenius-type rate equation
XI		the initial computing interval. If no XI is input, 0.0001220703125 will be used
ELE1		an array of $[2(\text{IMAX}) + 1]$ values used by integration scheme to control size of computing interval. $0.0 < \text{ELE1} \leq 64.0$
ELE2		an array of $[2(\text{IMAX}) + 1]$ values used by integration scheme to control size of computing interval. $\text{ELE2} < \text{ELE1}$
XPST		an array of x values at which physical space calculations are desired. They must be multiples of DELX. The program sets $\text{XPST}(1) = \text{DELX}$ and $\text{XPST}(\text{NXPST}) = [(x \text{ at ZSTERM}) + 100.0]$
NXPST		number of values in XPST array ≤ 100
IPF		PRINT ANSWERS every IPF integration; IPF = 5 unless input otherwise

APPENDIX A – Continued

FORTRAN name	Symbol	Description
CIMAX		maximum computing interval; if CIMAX is not input, 0.0625 will be used
TIMER		time, in decimal seconds, requested on JOB card. If case does not terminate in time estimated on JOB card, data for pickup will be stored on tape 13. If TIMER is not input, 3600.0 or 1 hour will be used
IPICKUP		= 1 to pickup case from tape 13 = 0 unless input
IBUG		an array of 15 integers which must be input as 0 to trigger debug printouts at critical points (see Program Listing

\$

With some cases, difficulties were encountered in starting the integration. When this condition occurred, the input quantities XI, ELE1, ELE2, and CIMAX were varied until the integration proceeded.

After reading in NAMELIST input, read in the IMAX species (10 spaces per species, 8 species per card) by Format (8A10) and the JMAX reactions by the same FORMAT using 20 spaces per reaction, 4 reactions per card. If the species and reactions are not read in, $IMAX/8 + JMAX/4$ blank cards must be put in the deck. If $(IMAX/8)$ and $(JMAX/4)$ are not whole numbers, they should be rounded to the next whole number.

Sample Input

A sample input follows:

```

SHOCK SHAPE NEQA      GROSE.12-17-68  7 SPECIES.14 REACTIONS      0000
$NAME1
M=0.
MUI(1)= 28.016.32.000.14.008.16.000.30.008.30.008.5.4862E-4.
CIINF(1)=0.768..232..0..0..0..0..0.
PINF=1.98E2.
TINF = 253.8.
VINP = 7.02E5.

```

APPENDIX A - Continued

```

R      = 8.31469E7.
GAMMA= 1.4.
THETA1(1)= 3392.14,2275.0,1.0,1.0,2739.0,3421.0,1.0.
GIL(1,1 )= 1.0,3.0,6.0,2.0,4*0..
GIL(1,2 )= 3.0,2.0,1.0,3.0,1.0,3.0,2*0..
GIL(1,3 )= 4.0,6.0,4.0,6.0,4*0..
GIL(1,4 )= 5.0,3.0,1.0,5.0,1.0,3*0..
GIL(1,5 )= 2.0,2.0,2.0,4.0,2.0,4.0,2.0,4..
GIL(1,6 )= 1.0,6.0,3.0,5*0..
GIL(1,7 )= 1.0,7*0..
DGENT(1)= 20*1.0.
EPSIIL(1, 1)= 0.0,71592.0,85343.0,99212.0, 4*0..
EPSIIL(1, 2)= 0.0,11342.0,18879.0,51385.0,52104.0,71026.0, 2*0..
EPSIIL(1, 3)= 0.0,27659.0,27670.0,41496.0, 4*0..
EPSIIL(1, 4)= 0.0, 228.0, 326.0,22831.0,48622.0, 3*0..
EPSIIL(1, 5)= 0.0, 174.0,63597.0,65381.0,76676.0,75361.0,87568.0,86359.0.
EPSIIL(1, 6)= 0.0,57528.0,84205.0, 5*0..
EPSIIL(1, 7)= 8*0..
LI(1)= 4.6,4.5,8.3,1.
FI(1)= 1.0,1.0,0.0,0.0,1.0,1.0,0.0.
DELHI(1)=0.0,0.0,4.707E12,2.4681E12,9.0073E11,1.0826E13,0.0.
DELI(1)= 114981.0,60500.0,0.0,0.0,76883.0,127698.0,0.0.
MJ(1)= 2.4,5.3,1.3,2.5,1.5,1.5,6.3.
MJ(11)= 6.3,0.0.
AJ(1)= 1.2E21,1.0E18,5.2E21,1.3E21,3.0E21,1.67E20,1.0E12,2.38E11,5.0E13,
1.11E13,9.1E24,4.79E23,1.8E21,2.17E11.
AJ(11)= 1.8E21,2.17E11,0.0.
BJ(1)= -1.5,-1.0,-1.5,-1.5,-1.5,-1.5,0.5,0.5,0.5,0.0,0.0,-2.5,-2.5,-1.5,0.12.
BJ(11)= -1.5,0.12,0.0.
EJ(1)= 59380.0,0.0, 75490.0,0.0, 113260.0,0.0, 3120.0, 19130.0, 38000.0,0.0.
EJ(11)= 0.0,31858.0,0.0.
NUIJ(1, 1)= 0.1,0.0,0.0,0.0,0.1.
NUIJ(1, 2)= 0.0,0.0,2.0,0.0,0.1.
NUIJ(1, 3)= 0.0,0.0,0.1,0.0,0.1.
NUIJ(1, 4)= 0.0,0.1,1.0,0.0,0.1.
NUIJ(1, 5)= 1.0,0.0,0.0,0.0,0.1.
NUIJ(1, 6)= 0.0,2.0,0.0,0.0,0.1.
NUIJ(1, 7)= 0.1,1.0,0.0,0.0,0.0.
NUIJ(1, 8)= 0.0,0.0,1.1,0.0,0.0.
NUIJ(1, 9)= 1.0,0.0,1.0,0.0,0.0.
NUIJ(1,10)= 0.0,1.0,0.1,0.0,0.0.
NUIJ(1,11)= 0.0,0.0,0.0,1.1,0.0.
NUIJ(1,12)= 0.0,0.1,1.0,0.0,0.0.
NUPIJ(1, 1)= 0.0,0.0,2.0,0.0,0.0.
NUPIJ(1, 2)= 0.1,0.0,0.0,0.0,0.0.
NUPIJ(1, 3)= 0.0,0.1,1.0,0.0,0.0.
NUPIJ(1, 4)= 0.0,0.0,0.1,0.0,0.0.
NUPIJ(1, 5)= 0.0,2.0,0.0,0.0,0.0.
NUPIJ(1, 6)= 1.0,0.0,0.0,0.0,0.0.
NUPIJ(1, 7)= 0.0,0.0,1.1,0.0,0.0.
NUPIJ(1, 8)= 0.1,1.0,0.0,0.0,0.0.
NUPIJ(1, 9)= 0.0,1.0,0.1,0.0,0.0.
NUPIJ(1,10)= 1.0,0.0,1.0,0.0,0.0.
NUPIJ(1,11)= 0.0,0.1,1.0,0.0,0.0.
NUPIJ(1,12)= 0.0,0.0,0.0,0.1,1.0.
AIJ(1, 1)= 6*1.0.
AIJ(1, 2)= 6*1.0.
AIJ(1, 3)= 6*1.0.
AIJ(1, 4)= 6*1.0.
AIJ(1, 5)= 6*1.0.
AIJ(1, 6)= 6*1.0.
AIJ(1, 7)= 7*0.
AIJ(1, 8)= 7*0.
AIJ(1, 9)= 7*0.
AIJ(1,10)= 7*0.

```

APPENDIX A - Continued

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AIJ(1,11)= 7*0,
AIJ(1,12)= 7*0,
ALPIK(1, 1)= 7*5.675E-4,
ALPIK(1, 2)= 7*1.443E-7,
ALPIK(1, 3)= 7*0,
ALPIK(1, 4)= 7*0,
ALPIK(1, 5)= 7*1.513E-4,
ALPIK(1, 6)= 7*1.513E-4,
ALPIK(1, 7)= 7*0.,
BETAIK(1, 1)=7*-.09952,
BETAIK(1, 2)=7*0.37177,
BETAIK(1, 3)=7*0.,
BETAIK(1, 4)=7*0.,
BETAIK(1, 5)=7*-.2226,
BETAIK(1, 6)=7*-.2226,
BETAIK(1, 7)=7*0,
SIGIK(1, 1)= 7*163.63,
SIGIK(1, 2)= 7*179.32,
SIGIK(1, 3)= 7*0,
SIGIK(1, 4)= 7*0,
SIGIK(1, 5)= 7*135.3,
SIGIK(1, 6)= 7*135.3,
SIGIK(1, 7)= 7*0,
IMAX=7,
JMAX=12,
CIMAX=.5,
ELE1(1)=42*64.,
ELE2(1)=42*1.0,
XI=.0625,
ZSTERM=1.145,
DELX=0.06, TCHECKT=0.3, HCHECKT=0.01, PHMAX=65.0,
EVI(1)=20*0.0,
NXPST=15, XPST(1)=.06,.12,.18,.24,.3,.36,.42,.48,.54,.6,.66,.72,.78,.84,1.0,
IPF=5, TIMER=240., IPICKUP=0,

```

\$

N2	O2	N	O	NO	NO+	E-
02 + M = 20 + M		20 + M = 02 + M		NO + M = N + O + M		N + O + M = NO + M
N2 + M = 2N + M		2N + M = N2 + M		N + O2 = NO + O		NO + O = N + O2
N2 + O = NO + N		NO + N = N2 + O		NO+ + E- = N + O		N + O = NO+ + E-

Tape Assignments

Tape 5, input, with buffer size 1001

Tape 6, output, with buffer size 1001

Tape 8, to save derivative of pressure at each x for each ψ

Tape 9, to save pressure at each x for each ψ

Tape 10, to save the shock geometry parameters x and corresponding z , r , R_c , $\cos \theta$, and $\sin \theta$

Tape 11, to save quantities behind the shock T_s , e_s , p_s , ρ_s , u_s , ψ_s , h_s , $(e_{v,i})_s (i = 1, \text{IMAX})$ at each x

Tape 12, to save physical space data

Tape 13, pickup tape

APPENDIX A – Continued

Operational Details

Program D1290 was written in FORTRAN IV language for the Control Data 6000 series digital computer under the Scope 3.0 operating system. The program requires a field length of 110 000₈. The sample case was completed in two passes on the Control Data 6600 computer to illustrate the pickup capability.

Programed STOPS

STOP 1, incorrect input
STOP 6, EOF 10 in main program
STOP 13, in SHOCKG
STOP 30, in CHECK when computing interval less than $1.0E - 15$
STOP 50, EOF 9 in FDPDX
STOP 66, in BASIC when no convergence on e iteration
STOP 301, in MAIN for error in XPST array or IZTERM .GT. 500
STOP 321, ITR1 stop in main program
STOP 422, in MAIN after pickup tape written
STOP 663, in MAIN when x is not equal to VARI(IPSI)
STOP 665, in MAIN after an integration attempt
STOP 670, when ac_i is negative

Pickup Tape

Under control of the input value TIMER, the estimated time on the JOB card and a REQUEST card, a pickup tape will be generated if the case does not terminate in the estimated time. A pickup may not be made before the $\psi = 0.0$ streamline integration has started.

Output

When no debug printouts are requested (IBUG array = 1), the printed output will contain:

- 1 ID information
- 2 a list of the IMAX species
- 3 a list of the JMAX reactions

APPENDIX A - Continued

- 4 a printout of the input quantities and those generated in the initialization section
- 5 the shock geometry x , z , r , R_c , $\cos \theta$, and $\sin \theta$
- 6 the free-stream quantities μ_∞ , ρ_∞ , a_∞ , M_∞ , $e_{i,\infty}$, e_∞ , $(e_{e,i})_\infty$, and $(e_{v,i})_\infty$ ($i = 1, \text{IMAX}$)
- 7 the quantities behind the shock T_s , e_s , p_s , ρ_s , u_s , ψ_s , h_s , and $(e_{v,i})_s$ ($i = 1, \text{IMAX}$) for each streamline ψ or each x distance along shock
- 8 IZTERM, the number of x values on the shock or the number of streamlines to be integrated
- 9 The following values are printed every IPF acceptable integration intervals:

IPSI streamline ID beginning with 2 for ψ at $x = \text{DELX}/5$

IX number of integration steps for streamline beginning with 1 at the shock

 $\left. \begin{matrix} x, h, \mu, p \\ \rho, u, T, e \end{matrix} \right\}$ for computing interval $\sum_{i=1}^{\text{IMAX}} c_i$

 c_i ($i=1, \text{IMAX}$) concentration

 $c_{m,i}$ ($i=1, \text{IMAX}$) molecular concentration

 $e_{v,i}$ ($i=1, \text{IMAX}$) vibrational energy

(IPSI=6) is used for the stagnation streamline, $\psi = 0.0$, and the streamline beginning at Δx
- 10 after all the streamlines have been computed, the physical space values r, y, z are printed at the x values given in the XPST array
- 11 after the initial conditions for a streamline are printed, the statement "——CHECKT= " appears. This number represents the elapsed time, in seconds, from start

APPENDIX A – Continued

- 12 other comments are printed to help the user follow the flow of the solution or to explain built-in remedial maneuvers to continue a solution which is in trouble
- 13 the IBUG debug printout options represent areas of difficulty during the development of the program. They may be helpful to the user for a closer examination of selected quantities and so have been left in the program.

Sample Output

A sample output follows:

SHOCK	SHAPE	NEQA	GROSE, 12-17-68	7 SPECIES, 14 REACTIONS	0000

	1	2	3	4	5	6	7
N ₂							
O ₂							
N ₂ O							
NO							
NO ₂							
E ⁻							

1	$O_2 + H = 2O + H$
2	$2O + H = O_2 + H$
3	$NO + H = N + O + H$
4	$N + C + M = NO + M$
5	$2N + M = 2N + M$
6	$2N + M = N_2 + M$
7	$N + O_2 = NO + O$
8	$NC + O = N + O_2$
9	$N_2 + O = NO + N$
10	$NO + N = N_2 + O$
11	$NO + E = N + O$
12	$N + O = NO + E$

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APPENDIX A - Continued

I= 1 (GIL(L,I),L=1,IMAX+1)	6.0000000E+00	2.0000000E+00	0.	0.	0.
1.0000000E+00 3.0000000E+00					
I= 1 (EPSIIL(L,I),L=1,IMAX+1)	8.5343000E+04	5.9212000E+04	0.	0.	0.
0. 7.1592000E+04					
I= 1 (AIJ(I,J),J=1,JMAX)	1.0000000E+00	1.0000000E+00	1.0000000E+00	1.0000000E+00	0.
1.0000000E+00 1.0000000E+00	0.	0.	0.	0.	
I= 1 (ALPIK(K,I),K=1,IMAX)	5.6750000E-04	5.6750000E-04	5.6750000E-04	5.6750000E-04	5.6750000E-04
5.6750000E-04 5.6750000E-04					
I= 1 (BETAIK(I),K=1,IMAX)	-9.9520000E-02	-9.9520000E-02	-9.9520000E-02	-9.9520000E-02	-9.9520000E-02
-9.9520000E-02 -9.9520000E-02					
I= 1 (SIGIK(K,I),K=1,IMAX)	1.6363000E+02	1.6363000E+02	1.6363000E+02	1.6363000E+02	1.6363000E+02
1.6363000E+02 1.6363000E+02					
I= 1 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
0. 0.	0.	0.	0.	0.	
I= 1 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
0. 0.	0.	0.	0.	0.	
I= 2 (GIL(L,I),L=1,IMAX+1)	1.0000000E+00	3.0000000E+00	1.0000000E+00	3.0000000E+00	0.
3.0000000E+00 2.0000000E+00					
I= 2 (EPSIIL(L,I),L=1,IMAX+1)	1.8879000E+04	5.1385000E+04	5.2104000E+04	7.1026000E+04	0.
0. 1.1342000E+04					
I= 2 (AIJ(I,J),J=1,JMAX)	1.0000000E+00	1.0000000E+00	1.0000000E+00	1.0000000E+00	0.
1.0000000E+00 1.0000000E+00	0.	0.	0.	0.	
I= 2 (ALPIK(K,I),K=1,IMAX)	1.4430000E-07	1.4430000E-07	1.4430000E-07	1.4430000E-07	1.4430000E-07
1.4430000E-07 1.4430000E-07					
I= 2 (BETAIK(I),K=1,IMAX)	3.7177000E-01	3.7177000E-01	3.7177000E-01	3.7177000E-01	3.7177000E-01
3.7177000E-01 3.7177000E-01					
I= 2 (SIGIK(K,I),K=1,IMAX)	1.7932000E+02	1.7932000E+02	1.7932000E+02	1.7932000E+02	1.7932000E+02
1.7932000E+02 1.7932000E+02					
I= 2 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
0. 0.	0.	0.	0.	0.	
I= 2 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
0. 0.	0.	0.	0.	0.	
I= 3 (GIL(L,I),L=1,IMAX+1)	4.0000000E+00	6.0000000E+00	0.	0.	0.
4.0000000E+00 6.0000000E+00					
I= 3 (EPSIIL(L,I),L=1,IMAX+1)	2.7670000E+04	4.1496000E+04	0.	0.	0.
0. 2.7659000E+04					

APPENDIX A - Continued

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[illegible]

APPENDIX A - Continued

I= 5 (BETAIK(K,I),K=1,IMAX)	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01
I= 5 (SIGIK(K,I),K=1,IMAX)	1.35300000E+02	1.35300000E+02	1.35300000E+02	1.35300000E+02	1.35300000E+02
I= 5 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
I= 5 (NUPIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
I= 5 (NUPIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
I= 6 (GIL(L,I),L=1,IPAX+1)	1.00000000E+00	0.	0.	0.	0.
I= 6 (EPSIIL(L,I),L=1,IPAX+1)	0.	0.	0.	0.	0.
I= 6 (ALIJ(I,J),J=1,JMAX)	1.00000000E+00	0.	0.	0.	0.
I= 6 (ALPIK(K,I),K=1,IMAX)	1.51300000E-04	1.51300000E-04	1.51300000E-04	1.51300000E-04	1.51300000E-04
I= 6 (BETAIK(K,I),K=1,IMAX)	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01	-2.22600000E-01
I= 6 (SIGIK(K,I),K=1,IMAX)	1.35300000E+02	1.35300000E+02	1.35300000E+02	1.35300000E+02	1.35300000E+02
I= 6 (NUIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
I= 6 (NUPIJ(J,I),J=1,JMAX)	0.	0.	0.	0.	0.
I= 7 (GIL(L,I),L=1,IPAX+1)	1.00000000E+00	0.	0.	0.	0.
I= 7 (EPSIIL(L,I),L=1,IPAX+1)	0.	0.	0.	0.	0.
I= 7 (ALIJ(I,J),J=1,JMAX)	0.	0.	0.	0.	0.
I= 7 (ALPIK(K,I),K=1,IMAX)	0.	0.	0.	0.	0.
I= 7 (BETAIK(K,I),K=1,IMAX)	0.	0.	0.	0.	0.
I= 7 (SIGIK(K,I),K=1,IMAX)	0.	0.	0.	0.	0.

APPENDIX A - Continued

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I= 7 (NULJ(J,I),J=1,JMAX)									
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
I= 8 (NULJ(J,I),J=1,JMAX)									
1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00	1.00000000E+00
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
END INPUT									
X	ZS	RS	RC	CGST	SINT				
0.	0.	0.	2.10921600E+00	0.	1.00000000E+00	1			
1.20000000E-02	4.68747616E-05	1.19998779E-02	2.10930975E+00	5.68914412E-03	9.99977777E-01	2			
2.40000000E-02	1.85091743E-04	2.35987784E-02	2.10958622E+00	1.13768982E-02	9.99912286E-01	3			
3.60000000E-02	3.77694702E-04	3.59570699E-02	2.10957149E+00	1.70638248E-02	9.99820981E-01	4			
4.80000000E-02	5.70257660E-04	4.79554154E-02	2.11035676E+00	2.27597513E-02	9.99729695E-01	5			
6.00000000E-02	9.87121805E-04	5.99869210E-02	2.11119117E+00	2.84280000E-02	9.99532435E-01	6			
1.20000000E-01	3.48580648E-03	1.19931853E-01	2.11161936E+00	5.67963502E-02	9.98350195E-01	7			
1.80000000E-01	8.96227244E-03	1.78662811E-01	2.12720253E+00	8.48621154E-02	9.95780042E-01	8			
2.40000000E-01	1.46866721E-02	2.39375523E-01	2.13871152E+00	1.12959267E-01	9.93094237E-01	9			
3.00000000E-01	2.63827066E-02	2.98732633E-01	2.15466264E+00	1.40453039E-01	9.89437704E-01	10			
3.60000000E-01	3.50371223E-02	3.57379120E-01	2.18028318E+00	1.67024407E-01	9.83842393E-01	11			
4.20000000E-01	4.74359740E-02	4.16025607E-01	2.20570372E+00	1.93595775E-01	9.78247083E-01	12			
4.80000000E-01	5.98348256E-02	4.74672095E-01	2.23112426E+00	2.20167143E-01	9.72651772E-01	13			
5.40000000E-01	7.23363773E-02	5.33318582E-01	2.25654479E+00	2.46738511E-01	9.67056461E-01	14			
6.00000000E-01	8.46325290E-02	5.91965069E-01	2.28156533E+00	2.73309879E-01	9.61461150E-01	15			
6.60000000E-01	1.07011744E-01	6.47142298E-01	2.31469388E+00	2.95590476E-01	9.52730755E-01	16			
7.20000000E-01	1.32327905E-01	7.01300184E-01	2.38866053E+00	3.16630418E-01	9.43077815E-01	17			
7.80000000E-01	1.57644066E-01	7.55457388E-01	2.44465169E+00	3.37626360E-01	9.33424864E-01	18			
8.40000000E-01	1.82960226E-01	8.05614592E-01	2.50124284E+00	3.58644301E-01	9.23771913E-01	19			
9.00000000E-01	2.08276387E-01	8.63771796E-01	2.55783400E+00	3.79662243E-01	9.14118962E-01	20			
9.60000000E-01	2.33592548E-01	9.17929000E-01	2.61442515E+00	4.00680185E-01	9.04466011E-01	21			
1.02000000E-00	2.58908708E-01	9.72086204E-01	2.67101631E+00	4.21698127E-01	8.94813060E-01	22			
1.08000000E-00	2.84224869E-01	1.02624341E+00	2.72760746E+00	4.42716068E-01	8.85160110E-01	23			
1.14000000E-00	3.09541030E-01	1.08040061E+00	2.78419861E+00	4.63734010E-01	8.75507159E-01	24			
1.20000000E-00	3.34857190E-01	1.13455782E+00	2.84078977E+00	4.84751952E-01	8.65854208E-01	25			
1.26000000E-00	3.60173351E-01	1.18871502E+00	2.89728092E+00	5.05769894E-01	8.56201257E-01	26			
1.32000000E-00	3.85485512E-01	1.24287222E+00	2.95357208E+00	5.26787835E-01	8.46548306E-01	27			
1.38000000E-00	4.12172446E-01	1.29598041E+00	3.01656607E+00	5.46921986E-01	8.36943558E-01	28			
1.44000000E-00	4.56753599E-01	1.33535953E+00	3.07722188E+00	5.55489530E-01	8.27965658E-01	29			
1.50000000E-00	5.01328171E-01	1.37473866E+00	3.15772218E+00	5.64057074E-01	8.18995758E-01	30			
1.56000000E-00	5.45905784E-01	1.41411779E+00	3.24003438E+00	5.72624619E-01	8.10021858E-01	31			
1.62000000E-00	5.90483396E-01	1.45349691E+00	3.32887828E+00	5.81192163E-01	8.01047958E-01	32			
1.68000000E-00	6.35061009E-01	1.49286704E+00	3.42234658E+00	5.89759707E-01	7.92074058E-01	33			
1.74000000E-00	6.7963621E-01	1.53225516E+00	3.51722188E+00	5.98327252E-01	7.83130158E-01	34			
1.80000000E-00	7.24216234E-01	1.57163429E+00	3.60350268E+00	6.06894796E-01	7.74126258E-01	35			
1.86000000E-00	7.68793846E-01	1.61101342E+00	3.69458788E+00	6.15462340E-01	7.65152358E-01	36			
1.92000000E-00	8.13371459E-01	1.65039254E+00	3.78416342E+00	6.24029844E-01	7.56178458E-01	37			
1.98000000E-00	8.57949071E-01	1.68977167E+00	3.87281709E+00	6.32597429E-01	7.47204558E-01	38			
2.04000000E-00	9.02526684E-01	1.72915080E+00	3.9628319E+00	6.41164973E-01	7.38230658E-01	39			
2.10000000E-00	9.47104256E-01	1.76852992E+00	4.05104329E+00	6.49732517E-01	7.29256758E-01	40			
2.16000000E-00	9.91681909E-01	1.80790905E+00	4.14851595E+00	6.58300061E-01	7.20282858E-01	41			

APPENDIX A - Continued

2.22000000E+00 1.03625952E+00 1.84728817E+00 4.99275149E+00 6.66867606E-01 7.11308958E-01 42
 2.28000000E+00 1.0803713E+00 1.88666739E+00 5.13350759E+00 6.75435150E-01 7.02335058E-01 43
 2.34000000E+00 1.12541475E+00 1.92604643E+00 5.2756369E+00 6.84002694E-01 6.93361158E-01 44
 2.40000000E+00 1.16995236E+00 1.96542555E+00 5.41621979E+00 6.92570238E-01 6.84387258E-01 45
 *** FREESTREAM QUANTITIES ***
 MUINF= 2.88492827E+01 RHQINF= 2.70683965E-07 AINF= 3.20011325E+04 MINF= 2.19367236E+01 EIINF= 5.76975408E+13
 EEIINF= 1.82888850E+09
 EVIINF= 0.
 1.57903727E+04 7.56528812E+05 0. 0. 1.56070331E+05 1.32695556E+04

*** QUANTITIES BEHIND SHECK ***
 TS PS RHQS US PSIS HS

1.76101270E+04 1.94671992E+11 1.18070770E+05 2.32631684E-06 0. 0. 2.45626372E+11
 IX= 1 EVIS= 4.73918161E+10 0. 0. 4.50982537E+10 4.42684304E+10 0.

1.76095021E+04 1.94862921E+11 1.18065372E+05 2.32629304E-06 3.99377917E+03 1.36811720E-05 2.45615501E+11
 IX= 2 EVIS= 4.73899672E+10 0. 0. 4.50965257E+10 4.4267044E+10 0.

1.76076600E+04 1.94636184E+11 1.18049461E+05 2.32622288E-06 7.98658257E+03 5.47202304E-05 2.45583454E+11
 IX= 3 EVIS= 4.73845170E+10 0. 0. 4.50914318E+10 4.42016162E+10 0.

1.76050932E+04 1.94798931E+11 1.18027292E+05 2.32612512E-06 1.19788050E+04 1.23113195E-04 2.45538893E+11
 IX= 4 EVIS= 4.73769228E+10 0. 0. 4.50843340E+10 4.41945264E+10 0.

1.76025265E+04 1.94761681E+11 1.18005125E+05 2.32602736E-06 1.59710274E+04 2.18661391E-04 2.45494156E+11
 IX= 5 EVIS= 4.73693287E+10 0. 0. 4.50772365E+10 4.41874369E+10 0.

1.75969803E+04 1.94681202E+11 1.17957231E+05 2.32581613E-06 1.99564560E+04 3.41887158E-04 2.45397692E+11
 IX= 6 EVIS= 4.73529195E+10 0. 0. 4.50619000E+10 4.41721177E+10 0.

1.75637484E+04 1.94199245E+11 1.17670402E+05 2.32455051E-06 3.98710378E+04 1.36659155E-03 2.44819957E+11
 IX= 7 EVIS= 4.72545978E+10 0. 0. 4.49700060E+10 4.40803277E+10 0.

1.74915493E+04 1.93153742E+11 1.17048101E+05 2.32180132E-06 5.95732050E+04 3.06679722E-03 2.43566638E+11
 IX= 8 EVIS= 4.70409030E+10 0. 0. 4.47703616E+10 4.38899106E+10 0.

1.74161678E+04 1.92064499E+11 1.16399640E+05 2.31893191E-06 7.92576721E+04 5.44413801E-03 2.42259867E+11
 IX= 9 EVIS= 4.68175732E+10 0. 0. 4.45619208E+10 4.36727091E+10 0.

APPENDIX A - Continued

1.73136478E+04 IX= 10 EVIS=	1.90587014E+11	1.15519835E+05	2.31503169E-06	9.85980337E+04	8.47681147E-03	2.42486997E+11
4.65146763E+10	4.20958508E+10	C.	C.	4.42784441E+10	4.33895611E+10	0.
1.71565557E+04 IX= 11 EVIS=	1.88338302E+11	1.14180306E+05	2.30977914E-06	1.17251134E+05	1.21346707E-02	2.37786719E+11
4.60512682E+10	4.16894161E+10	C.	C.	4.38453121E+10	4.29569390E+10	0.
1.70006191E+04 IX= 12 EVIS=	1.86104350E+11	1.12848976E+05	2.30314798E-06	1.35904234E+05	1.64440873E-02	2.35102060E+11
4.55886791E+10	4.12836865E+10	C.	C.	4.34129366E+10	4.25250818E+10	0.
1.68444941E+04 IX= 13 EVIS=	1.83685200E+11	1.11525859E+05	2.29724101E-06	1.54557334E+05	2.14070611E-02	2.32432939E+11
4.51268741E+10	4.08786311E+10	C.	C.	4.29812848E+10	4.20939572E+10	0.
1.66886132E+04 IX= 14 EVIS=	1.81680890E+11	1.10210966E+05	2.29136100E-06	1.73210435E+05	2.70235921E-02	2.29779363E+11
4.46658199E+10	4.04742202E+10	C.	C.	4.25503254E+10	4.16635339E+10	0.
1.65329654E+04 IX= 15 EVIS=	1.79491459E+11	1.08904310E+05	2.28551075E-06	1.91863535E+05	3.32936805E-02	2.27141337E+11
4.34885878E+10	4.00704257E+10	C.	C.	4.21200285E+10	4.12337823E+10	0.
1.62905487E+04 IX= 16 EVIS=	1.76105087E+11	1.06882010E+05	2.27644864E-06	2.07504514E+05	3.97896514E-02	2.23056293E+11
4.26977620E+10	3.94415524E+10	C.	C.	4.14458915E+10	4.05645153E+10	0.
1.60231030E+04 IX= 17 EVIS=	1.72403293E+11	1.04669434E+05	2.26653385E-06	2.22259109E+05	4.67280386E-02	2.18583690E+11
4.19087358E+10	3.87477844E+10	C.	C.	4.07106186E+10	3.98262327E+10	0.
1.57562326E+04 IX= 18 EVIS=	1.68746203E+11	1.02481509E+05	2.25674289E-06	2.37013704E+05	5.42237553E-02	2.14157450E+11
4.11214044E+10	3.80555477E+10	C.	C.	3.99729961E+10	3.90896316E+10	0.
1.54899007E+04 IX= 19 EVIS=	1.65133952E+11	1.00318277E+05	2.24708959E-06	2.51768300E+05	6.22768016E-02	2.09777600E+11
4.11214044E+10	3.73647482E+10	C.	C.	3.92369245E+10	3.83546144E+10	0.
1.52240773E+04 IX= 20 EVIS=	1.61566652E+11	9.81797769E+04	2.23758745E-06	2.66522895E+05	7.08871775E-02	2.05444167E+11
4.03356843E+10	3.66753105E+10	C.	C.	3.85023242E+10	3.76211031E+10	0.
1.49587404E+04 IX= 21 EVIS=	1.58044390E+11	9.60660374E+04	2.22824946E-06	2.81277490E+05	8.00548830E-02	2.01157174E+11
3.95515149E+10	3.55671788E+10	C.	C.	3.77691370E+10	3.68890414E+10	0.

APPENDIX A - Continued

1.46938758E+04 IX= 22 EVIS=	1.54567225E+11	5.39770798E+04	2.21908807E-06	2.96032085E+05	8.97799182E-02	1.96916639E+11
3.67688606E+10	3.53003194E+10	0.	0.	3.70373276E+10	3.61583959E+10	0.
1.44294786E+04 IX= 23 EVIS=	1.51135187E+11	9.19129162E+04	2.21011497E-06	3.10786680E+05	1.00062283E-01	1.92722578E+11
3.76877120E+10	3.46147210E+10	0.	0.	3.63068855E+10	3.54291580E+10	0.
1.41655528E+04 IX= 24 EVIS=	1.47748276E+11	8.98735454E+04	2.20134101E-06	3.25541275E+05	1.10901977E-01	1.88575003E+11
3.72080878E+10	3.39203571E+10	0.	0.	3.5578262E+10	3.47013453E+10	0.
1.39021126E+04 IX= 25 EVIS=	1.44406458E+11	8.78585721E+04	2.19277603E-06	3.40295870E+05	1.22299001E-01	1.84473921E+11
3.56536363E+10	3.32473869E+10	0.	0.	3.48501925E+10	3.39750029E+10	0.
1.36391922E+04 IX= 26 EVIS=	1.41105665E+11	8.58651662E+04	2.18442868E-06	3.55050465E+05	1.34253355E-01	1.80419333E+11
3.46785991E+10	3.25657563E+10	0.	0.	3.41240560E+10	3.32502048E+10	0.
1.33767668E+04 IX= 27 EVIS=	1.3757794E+11	8.39041025E+04	2.17630632E-06	3.69805060E+05	1.46765038E-01	1.76411238E+11
3.48785991E+10	3.18855989E+10	0.	0.	3.33995182E+10	3.25270547E+10	0.
1.31163079E+04 IX= 28 EVIS=	1.34666607E+11	8.19733386E+04	2.16845362E-06	3.83939234E+05	1.59575612E-01	1.72469292E+11
3.41101217E+10	3.12104212E+10	0.	0.	3.26803153E+10	3.18092842E+10	0.
1.28735059E+04 IX= 29 EVIS=	1.31724929E+11	8.01915008E+04	2.16132692E-06	3.89953650E+05	1.69420543E-01	1.68827831E+11
3.33936034E+10	3.05611480E+10	0.	0.	3.20100390E+10	3.11403948E+10	0.
1.26313174E+04 IX= 30 EVIS=	1.28821627E+11	7.84308859E+04	2.15440541E-06	3.95968066E+05	1.79560141E-01	1.65226514E+11
3.26790512E+10	2.95535262E+10	0.	0.	3.13615512E+10	3.04733434E+10	0.
1.23898046E+04 IX= 31 EVIS=	1.25556503E+11	7.66914644E+04	2.14768968E-06	4.01982482E+05	1.89994476E-01	1.61665323E+11
3.19666564E+10	2.93277203E+10	0.	0.	3.06750286E+10	2.98083085E+10	0.
1.21490376E+04 IX= 32 EVIS=	1.23129331E+11	7.49731683E+04	2.14117885E-06	4.07996858E+05	2.00723339E-01	1.58144233E+11
3.12566340E+10	2.87039152E+10	0.	0.	3.00106654E+10	2.91454911E+10	0.
1.19090940E+04 IX= 33 EVIS=	1.20339858E+11	7.32759216E+04	2.13487045E-06	4.14011314E+05	2.11746939E-01	1.54663215E+11
3.05492213E+10	2.808223150E+10	0.	0.	2.93486930E+10	2.84851128E+10	0.
1.16700581E+04 IX= 34 EVIS=	1.17587807E+11	7.15996405E+04	2.12876039E-06	4.20025731E+05	2.23065206E-01	1.51222236E+11
2.98446765E+10	2.74631423E+10	0.	0.	2.86853380E+10	2.78274147E+10	0.

APPENDIX A - Continued

1.14320209E+04 IX= 35 EVIS= 2.91432769E+10	1.14872880E+11 2.68466364E+10	6.99442345E+04 0.	2.12284296E-06 0.	4.26040147E+05 2.80328608E+10	2.34678140E-01 2.7172659E+10	1.47821260E+11 0.
1.11950789E+04 IX= 36 EVIS= 2.84453168E+10	1.12194760E+11 2.62230509E+10	6.83096066E+04 0.	2.11711077E-06 0.	4.32054563E+05 2.73795337E+10	2.46585742E-01 2.65211113E+10	1.44460246E+11 0.
1.09593333E+04 IX= 37 EVIS= 2.77511049E+10	1.09593112E+11 2.56226521E+10	6.66956546E+04 0.	2.11155483E-06 0.	4.38068979E+05 2.67296422E+10	2.58788010E-01 2.58730692E+10	1.41139151E+11 0.
1.07248890E+04 IX= 38 EVIS= 2.70609614E+10	1.06547566E+11 2.50157165E+10	6.51022721E+04 0.	2.10616454E-06 0.	4.44083395E+05 2.60834826E+10	2.71284946E-01 2.52288287E+10	1.37857931E+11 0.
1.04918540E+04 IX= 39 EVIS= 2.63752152E+10	1.04377824E+11 2.44125277E+10	6.35293490E+04 0.	2.10092779E-06 0.	4.50097811E+05 2.54413550E+10	2.84076549E-01 2.45886970E+10	1.34616536E+11 0.
1.02605550E+04 IX= 40 EVIS= 2.56948397E+10	1.01845833E+11 2.38139363E+10	6.19775081E+04 0.	2.09581147E-06 0.	4.56112227E+05 2.48041791E+10	2.97162820E-01 2.39535829E+10	1.31417915E+11 0.
1.00306336E+04 IX= 41 EVIS= 2.50187927E+10	9.93461194E+10 2.32190194E+10	6.0450483E+04 0.	2.09084250E-06 0.	4.62126643E+05 2.41709630E+10	3.10543757E-01 2.33225137E+10	1.28255541E+11 0.
9.80245541E+03 IX= 42 EVIS= 2.43481628E+10	9.68811281E+10 2.26287286E+10	5.89327281E+04 0.	2.08598234E-06 0.	4.68141059E+05 2.35427259E+10	3.24219362E-01 2.26965059E+10	1.25132915E+11 0.
9.57612792E+03 IX= 43 EVIS= 2.36832795E+10	9.44504916E+10 2.20433473E+10	5.74404342E+04 0.	2.08121397E-06 0.	4.74155475E+05 2.29197721E+10	3.38189633E-01 2.20758672E+10	1.22049977E+11 0.
9.35175595E+03 IX= 44 EVIS= 2.30244647E+10	9.20538501E+10 2.14631521E+10	5.59680556E+04 0.	2.07651949E-06 0.	4.80169891E+05 2.23023988E+10	3.52454573E-01 2.14608584E+10	1.19006670E+11 0.
9.12944068E+03 IX= 45 EVIS= 2.23720301E+10	8.96908562E+10 2.08884107E+10	5.45154852E+04 0.	2.07188033E-06 0.	4.86184307E+05 2.16908931E+10	3.67014179E-01 2.08518905E+10	1.16002938E+11 0.

XXXXX ITR= 13 NAPST= 15 XXXXX

IZTERM= 45

APPENDIX A - Continued

XXXXXXXXXXXXXXXXXX

2 1 X= 1.200000000-02 H= 2.456155010+11 MU= 2.88492827E+01 P= 1.18065372E+05 RHO= 2.32629304E-06
 U= 3.99377917E+03 T= 1.76095021E+04 E= 1.94862921E+11 CI(4)= 0. SUM(CI)= 1.00000000E+00
 CI(1)= 7.680000000-01 CI(2)= 2.320000000-01 CI(3)= 0. CI(5)= 0.
 CI(6)= 0. CI(7)= 0. CI(8)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 7.90842701E-01 CM(2)= 2.09157299E-01 CM(3)= 0. CM(6)= 0.
 CM(7)= 0. CM(8)= 0. EVI(4)= 0. EVI(5)= 4.509652570+10
 EVI(1)= 4.738996720+10 EVI(2)= 4.286349660+10 EVI(3)= 0. EVI(6)= 4.420670440+10 EVI(7)= 0. EVI(8)=

-----CHECK= 4.80250000E+01

2 6 X= 3.153125000-02 H= 2.456123350+11 MU= 2.07502764E+01 P= 1.18022305E+05 RHO= 2.81818299E-06
 U= 5.29848106E+03 T= 1.04513501E+04 E= 2.03733470E+11 CI(4)= 0. SUM(CI)= 9.99888171E-01
 CI(1)= 5.55273186D-01 CI(2)= 1.79584524D-03 CI(3)= 1.92089449D-01 CI(5)= 3.65880631D-02
 CI(6)= 1.21096398D-03 CI(7)= 2.21393982D-08 CI(8)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 4.11267565E-01 CM(2)= 1.16450891E-03 CM(3)= 2.84545199E-01 CM(6)= 0.
 CM(7)= 8.37371279E-04 CM(8)= 0. EVI(4)= 0. EVI(5)= 2.532978940+10
 EVI(1)= 2.62560750D+10 EVI(2)= 2.430771840+10 EVI(3)= 0. EVI(6)= 2.44774826D+10 EVI(7)= 0. EVI(8)=

2 11 X= 6.27812500D-02 H= 2.455942650+11 MU= 1.98840345E+01 P= 1.17884762E+05 RHO= 3.08842635E-06
 U= 8.01337358E+03 T= 9.12806804E+03 E= 2.07424418E+11 CI(4)= 0. SUM(CI)= 9.99888171E-01
 CI(1)= 5.09826645D-01 CI(2)= 7.71561894D-04 CI(3)= 2.43596931D-01 CI(5)= 2.33738066D-02
 CI(6)= 1.48251385D-03 CI(7)= 2.71039971D-08 CI(8)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 3.61845030E-01 CM(2)= 4.79678654E-04 CM(3)= 3.45780252E-01 CM(6)= 0.
 CM(7)= 9.82349921E-04 CM(8)= 0. EVI(4)= 0. EVI(5)= 1.54880557E-02
 EVI(1)= 2.23680029D+10 EVI(2)= 2.08848625D+10 EVI(3)= 0. EVI(6)= 2.16871182D+10
 EVI(7)= 0. EVI(8)=

XXXXXXXXXXXXXXXXXX

3 1 X= 2.400000000-02 H= 2.45583454D+11 MU= 2.88492827E+01 P= 1.18049461E+05 RHO= 2.32622288E-06
 U= 7.98638257E+03 T= 1.76076600E+04 E= 1.94836184E+11 CI(4)= 0. SUM(CI)= 1.00000000E+00
 CI(1)= 7.680000000-01 CI(2)= 2.320000000-01 CI(3)= 0. CI(5)= 0.
 CI(6)= 0. CI(7)= 0. CI(8)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 7.90842701E-01 CM(2)= 2.09157299E-01 CM(3)= 0. CM(6)= 0.
 CM(7)= 0. CM(8)= 0. EVI(4)= 0. EVI(5)= 4.509143180+10
 EVI(1)= 4.73845170D+10 EVI(2)= 4.28587149D+10 EVI(3)= 0. EVI(6)= 4.42016162D+10 EVI(7)= 0. EVI(8)=

-----CHECK= 5.42410000E+01

3 6 X= 6.30625000E-02 H= 2.45561095D+11 MU= 2.07531671E+01 P= 1.17889130E+05 RHO= 2.81578504E-06
 U= 1.14280046E+04 T= 1.04499108E+04 E= 2.03693862E+11 CI(4)= 0. SUM(CI)= 9.99839924E-01
 CI(1)= 5.55128647D-03 CI(2)= 1.79530601D-03 CI(3)= 1.92057323D-01 CI(5)= 3.65759165D-02
 CI(6)= 1.21133447D-03 CI(7)= 2.21461715D-08 CI(8)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 4.11217788E-01 CM(2)= 1.16432143E-03 CM(3)= 2.84537244E-01 CM(6)= 0.
 CM(7)= 8.3744153E-04 CM(8)= 0. EVI(4)= 0. EVI(5)= 2.52954580E-02
 EVI(1)= 2.62518178D+10 EVI(2)= 2.43039728D+10 EVI(3)= 0. EVI(6)= 2.53258023D+10
 EVI(7)= 0. EVI(8)=

APPENDIX A - Continued

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XXXXXXXXXXXXXXXXXXXX
4 1 X= 3.6000000000-02 MU= 2.88492827E+01 P= 1.18027292E+05 RHO= 2.32612512E-06
U= 1.19788050E+C4 E= 1.94798931E+11 CI= 4)= 0. SUM(CI)= 1.00000000E+00
CI( 1)= 7.6800000000-01 CI( 3)= 0. CI( 4)= 0. CI( 5)= 0.
CI( 6)= 0. CM( 4)= 0. CM( 5)= 0.
CM( 1)= 7.90842701E-01 CM( 3)= 0. CM( 4)= 0. CM( 5)= 0.
CM( 6)= 0. CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 4.508433400+10
EVI( 1)= 4.737652280+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 4.508433400+10
EVI( 6)= 4.419452640+10 EVI( 7)= 0. EVI( 8)= 0.

-----CHECK1= 5.74630000E+01
4 5 X= 6.7250000000-02 MU= 2.15266421E+01 P= 1.17868660E+05 RHO= 2.63390585E-06
U= 1.52294001E+C4 E= 2.00759884E+11 CI= 4)= 0. SUM(CI)= 1.00181248E+00
CI( 1)= 5.365566640-01 CI( 3)= 1.492735330-01 CI( 4)= 2.043258220-01 CI( 5)= 4.6866634010-02
CI( 6)= 6.350615240-04 CI( 7)= 1.161048570-08 CI( 8)= 2.25394483E-01 CM( 4)= 2.74903053E-01 CM( 5)= 3.36201990E-02
CM( 1)= 4.58375993E-01 CM( 3)= 4.55569920E-04 CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 2.845711920+10
CM( 6)= 4.55569920E-04 CM( 7)= 2.724506700+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 2.845711920+10
EVI( 1)= 2.59655890+10 EVI( 2)= 2.724506700+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 2.845711920+10
EVI( 6)= 2.759579570+10 EVI( 7)= 0. EVI( 8)= 0.

XXXXXXXXXXXXXXXXXXXX
5 1 X= 4.8000000000-C2 MU= 2.88492827E+01 P= 1.18005125E+05 RHO= 2.32602736E-06
U= 1.59710274E+C4 E= 1.94761681E+11 CI= 4)= 0. SUM(CI)= 1.00000000E+00
CI( 1)= 7.6800000000-01 CI( 3)= 0. CI( 4)= 0. CI( 5)= 0.
CI( 6)= 0. CM( 4)= 0. CM( 5)= 0.
CM( 1)= 7.90842701E-01 CM( 3)= 0. CM( 4)= 0. CM( 5)= 0.
CM( 6)= 0. CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 4.507723650+10
EVI( 1)= 4.736932870+10 EVI( 2)= 4.284539490+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 4.507723650+10
EVI( 6)= 4.418743690+10 EVI( 7)= 0. EVI( 8)= 0.

-----CHECK1= 6.02130000E+01
5 2 X= 6.3625000000-02 MU= 2.32749724E+01 P= 1.17910793E+05 RHO= 2.38810443E-06
U= 1.69707198E+C4 E= 1.96108149E+11 CI= 4)= 1.56250000E-02 SUM(CI)= 1.00549289E+00
CI( 1)= 6.679601C90-01 CI( 3)= 7.963689280-02 CI( 4)= 1.688851920-01 CI( 5)= 4.608505950-02
CI( 6)= 1.384366900-04 CI( 7)= 2.530962980-02 CI( 8)= 1.32320566E-01 CM( 4)= 2.45674887E-01 CM( 5)= 3.57447511E-02
CM( 1)= 5.34924084E-01 CM( 3)= 3.11209624E-02 CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 3.462651590+10
CM( 6)= 1.07375038E-04 CM( 7)= 1.07375038E-04 CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 3.462651590+10
EVI( 1)= 3.619087110+10 EVI( 2)= 3.303742260+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 3.462651590+10
EVI( 6)= 3.3751173320+10 EVI( 7)= 0. EVI( 8)= 0.

-----CHECK1= 6.02130000E+01
XXXXXXXXXXXXXXXXXXXX
PSI=0.000 STREAMLINE--
----- CHECK1= 6.09430000E+01 -----
6 6 X= 6.0000000000-02 MU= 2.88492827E+01 P= 1.17903357E+05 RHO= 3.19199053E-06
U= 6.48834434E+C3 E= 2.08668071E+11 CI= 4)= 6.25000000E-02 SUM(CI)= 9.99970928E-01
CI( 1)= 4.947270040-01 CI( 3)= 2.607786660-01 CI( 4)= 2.234888770-01 CI( 5)= 1.897262540-02
CI( 6)= 1.572916790-03 CI( 7)= 2.875678520-08 CI( 8)= 5.370700064E-01 CM( 4)= 4.02968362E-01 CM( 5)= 1.82400237E-02
CM( 1)= 5.09441719E-01 CM( 2)= 3.88392607E-04 CM( 3)= 5.370700064E-01 CM( 4)= 4.02968362E-01 CM( 5)= 1.82400237E-02
CM( 6)= 1.51218079E-03 CM( 7)= 1.51218079E-03 CM( 8)= 0. EVI( 4)= 0. EVI( 5)= 2.047570150+10
EVI( 1)= 2.107586570+10 EVI( 2)= 1.974607940+10 EVI( 3)= 0. EVI( 4)= 0. EVI( 5)= 2.047570150+10
EVI( 6)= 1.964204030+10 EVI( 7)= 0. EVI( 8)= 0.

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APPENDIX A - Continued

6	11	X= 9.906250000-02	H= 2.455554670+11	MU= 1.942403633E+01	P= 1.176119233E+05	RHO= 3.27099871E-06
		Y= 1.19083982E+04	T= 8.39372372E+03	E= 2.09599505E+11	CI= 7.8125000E-03	SUM(CI)= 1.00012796E+02
		U(1)= 4.4642906290-01	CI(1)= 4.141022200-04	CI(3)= 2.725622010-01	CI(4)= 2.253506460-01	CI(5)= 1.583170630-02
		CI(6)= 1.278548990-03	CI(7)= 2.337501830-08	CI(8)= 2.378500505E-01	CI(9)= 1.02478028E-02	CI(10)= 1.9695337880+10
		CM(1)= 3.35768595E-01	CM(2)= 2.51360887E-34	CM(3)= 3.78500505E-01	CM(4)= 2.73576576E-01	CM(5)= 1.02478028E-02
		CM(6)= 8.27598589E-04	CM(7)= 8.27598589E-04	CM(8)= 2.73576576E-01	CM(9)= 1.02478028E-02	CM(10)= 1.9695337880+10
		EV(1)= 2.023322740+10	EV(2)= 1.900298550+10	EV(3)= 0.	EV(4)= 0.	EV(5)= 1.9695337880+10
		EV(6)= 1.885549190+10	EV(7)= 0.	EV(8)= 2.73576576E-01	EV(9)= 1.02478028E-02	EV(10)= 1.9695337880+10

	16	6
X=	1.381250000-01	H= 2.455036230+11
U=	1.56683972E+04	T= 8.25042446E+03
CI(1)=	4.788490510-04	CI(2)= 3.593560920-04
CI(6)=	2.18663110-03	CI(7)= 2.228015720-08
CI(1)=	3.20523074E-04	CI(2)= 2.17120776E-04
CI(6)=	7.85186753E-04	CI(7)= 7.85186753E-04
EV(1)=	1.979621200+10	EV(2)= 1.861746050+10
EV(6)=	1.844758200+10	EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.
		EV(8)= 0.
		EV(4)= 0.
		EV(5)= 1.927540860+10
		EV(3)= 0.
		EV(1)= 0.
		EV(2)= 0.
		EV(7)= 0.

6	21	X= 1.771875000-01 U= 4.70593335E+04 CII 1)= 2.59555860-01 CII 6)= 1.185449420-03 CMI 1)= 3.27234965E-01 CMI 6)= 7.61569612E-04 EVI 1)= 1.950909520+10 EVI 6)= 1.817959060+10	H= 2.4540464340+11 T= 8.152294359E+03 CII 2)= 3.270427810-04 CII 7)= 2.167252920-08 CMI 2)= 1.97023586E-04 CMI 7)= 7.61569612E-04 EVI 2)= 1.836411450+10 EVI 7)= 0.	MU= 1.92780735E+01 E= 2.102833537E+11 CII 3)= 2.827983930-01 CII 8)= 1.71252920-08 CMI 3)= 3.89152475E-01 CMI 8)= 7.61569612E-04 EVI 3)= 0.	P= 1.16611571E+05 CI= 7.8125000E-03 CII 4)= 2.266934110-31 CII 5)= 1.35643050-02 CMI 4)= 2.73138265E-31 CMI 5)= 8.71413216E-13 EVI 4)= 0. EVI 5)= 1.900602120+10	RHO= 3.31649502E-36 SUM(CII)= 1.00312521E+02 CII 5)= 1.35643050-02 CMI 5)= 8.71413216E-13 EVI 5)= 1.900602120+10
---	----	---	--	---	---	--

6	26	X= 2.7093735000-01 U= 3.552453505E+03 Y= 4.711859720-01 C1(1)= 1.1388767240-03 C1(6)= 1.33007166E-01 C1(11)= 3.23007166E-01 C1(6)= 7.28902788E-04 C1(11)= 1.508533710+10 EVI(6)= 1.778466160+10 EVI(11)= 0.	H= 2.449953620+11 T= 8.00740135E+03 Y= 2.853175590-04 C1(1)= 2.082165820-08 C1(7)= 1.71238618E-04 C1(2)= 7.28902788E-04 C1(7)= 1.79901101C+10 EVI(2)= 0.	MU= 1.92055140E+01 E= 2.10328724E+11 C1(3)= 2.877367600-01 C1(8)= 3.94458312E-01 C1(3)= 7.27932421E-01 C1(8)= 0.	P= 1.14868117E+05 CI= 3.12500000E-02 CI(4)= 2.273783850-01 CM(4)= 2.72932421E-01 CM(5)= 7.93305662E-03 EVI(4)= 0.	RHO= 3.31350611E-06 SUM(CI)= 1.00012049E+00 CI(5)= 1.23951467D-02 CM(5)= 1.8608337C+0+10 EVI(5)= 0.
---	----	---	--	---	--	--

6	31	X= 4.27187500D-01 Y= 6.047163638E+03 Z= 4.67947259D-01 C1(1)= 1.08973328D-03 C1(6)= 3.19877495E-01 CM(1)= 6.95413621E-04 CM(6)= 1.8558897D+10 EVI(1)= 1.73300238D+10	H= 2.43801304D+11 T= 7.84097361E+03 V= 2.46885641D-04 C1(7)= 1.99230030D-08 C1(8)= 1.48540785E-04 CM(7)= 6.95419621E-04 CM(8)= 1.75663966C+10 EVI(7)= 0. EVI(8)= 0.	MU= 1.91497794E+01 E= 2.05756375E+11 C1(3)= 2.91473911D-01 C1(8)= 3.98462386E-01 CM(3)= 3.98462386E-01 CM(8)= 3.98462386E-01 EVI(3)= 0. EVI(8)= 0.	P= 1.10172548E+35 CI= 3.12500000E-32 C1(4)= 2.28013057D-31 CM(4)= 2.72899984E-31 CM(5)= 7.22335545E-33 EVI(4)= 0. EVI(5)= 1.81518003D+10	RHO= 3.236399277E-06 SUM(C1(1)= 1.00911897E+00 C1(5)= 1.13191095D-22
---	----	--	---	---	---	--

6	36	$ \begin{aligned} &X = 5.834375000-01 & H = 2.421618030+11 & MU = 1.91224627E+01 & P = 1.04767916E+05 & RHO = 3.13163581E-06 \\ &U = 8.32414772E+04 & Y = 7.69404665E+03 & E = 2.08707109E+11 & CI = 3.12500000E-32 & SUM(CI) = 1.06011849E+00 \\ &U(1) = 4.66648780E-01 & CI(1) = 2.23180344D-04 & CI(3) = 2.93190414D-01 & CI(4) = 2.28485128D-01 & CI(5) = 1.05234916D-12 \\ &CI(6) = 1.04747302D-03 & CI(7) = 1.91503816D-08 & CI(8) = 3.1 & CM(4) = 2.73074896E-01 & CM(5) = 6.70604756E-03 \\ &CI(11) = 3.185113489E-01 & CM(2) = 1.33367432E-04 & CM(3) = 4.00237205E-01 & EVI(4) = 0. & EVI(5) = 1.77488766D+10 \\ &CM(6) = 6.67497463E-04 & CM(7) = 6.67497463E-04 & CM(8) = 3.0. & EVI(4) = 0. & EVI(5) = 1.77488766D+10 \\ &EVI(1) = 1.81696917D+10 & EVI(2) = 1.71815839D+10 & EVI(3) = 0. & EVI(4) = 0. & EVI(5) = 1.77488766D+10 \\ &EVI(6) = 1.69294254D+10 & EVI(7) = 0. & EVI(8) = 0. & EVI(4) = 0. & EVI(5) = 1.77488766D+10 \end{aligned} $
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APPENDIX A - Continued

6	41	X= 7.39687500D+01 U= 1.05661956E+05 CII(1)= 4.66115556D-01 CII(6)= 1.00649252D-03 CII(7)= 3.17885816E-01 CII(8)= 6.40853737E-04 CII(9)= 1.77085032D+10 EVI(6)= 1.64985729D+10 EVI(7)= 0.	H= 2.40044148D+11 T= 7.53608424E+03 CII(2)= 2.01022771D-04 CII(7)= 1.84011573D-08 CII(8)= 1.20027482E-04 CII(9)= 6.40853737E-04 EVI(2)= 1.67741316D+10 EVI(7)= 0.	MU= 1.91066884E+01 E= 2.07249329E+11 CII(3)= 2.94069684D-01 CII(8)= 4.01106354E-01 CII(9)= 0. EVI(3)= 0. EVI(8)=	P= 9.75016084E+04 CI= 3.12500000E-02 CII(4)= 2.28907018D-01 CII(5)= 9.81382156D-03 CII(6)= 2.73353440E-01 CII(7)= 6.24865469E-03 EVI(4)= 0. EVI(5)= 1.73158245D+10	RHO= 2.97307966E-06 SUM(CI)= 1.00011761E+00 CII(5)= 9.81382156D-03 CII(6)= 2.73353440E-01 CII(7)= 6.24865469E-03 EVI(5)= 1.73158245D+10
6	46	X= 9.95937500D-01 U= 1.28297085E+05 CII(1)= 4.66121034D-01 CII(6)= 9.62828309D-04 CII(7)= 3.17740331E-01 CII(8)= 6.12634358E-04 CII(9)= 1.71815148D+10 EVI(6)= 1.60074854D+10 EVI(7)= 0.	H= 2.37396301D+11 T= 7.35554186E+03 CII(2)= 1.79055810D-04 CII(7)= 1.75992116D-08 CII(8)= 1.06861208E-04 CII(9)= 6.12634358E-04 EVI(2)= 1.63087056D+10 EVI(7)= 0.	MU= 1.90376430E+01 E= 2.05371904E+11 CII(3)= 2.94427539D-01 CII(8)= 4.01404343E-01 CII(9)= 0. EVI(3)= 0. EVI(8)=	P= 8.98280434E+04 CI= 3.12500000E-02 CII(4)= 2.29333935D-01 CII(5)= 9.08699018D-03 CII(6)= 2.73740068E-01 CII(7)= 5.78312765E-03 EVI(4)= 0. EVI(5)= 1.68212320D+10	RHO= 2.80498781E-06 SUM(CI)= 1.00011662E+00 CII(5)= 9.08699018D-03 CII(6)= 2.73740068E-01 CII(7)= 5.78312765E-03 EVI(5)= 1.68212320D+10
6	51	X= 1.05218750D+00 U= 1.48672957E+C5 CII(1)= 4.66406783D-01 CII(6)= 9.17772528D-04 CII(7)= 3.17847542E-01 CII(8)= 5.83926426E-04 CII(9)= 1.66402651D+10 EVI(6)= 1.55015483D+10 EVI(7)= 0.	H= 2.34574548D+11 T= 7.16969265E+03 CII(2)= 1.58253446D-04 CII(7)= 1.67791377D-08 CII(8)= 9.44198538E-05 CII(9)= 5.83926426E-04 EVI(2)= 1.58297361D+10 EVI(7)= 0.	MU= 1.90323825E+01 E= 2.03350697E+11 CII(3)= 2.94499028D-01 CII(8)= 4.01391212E-01 CII(9)= 0. EVI(3)= 0. EVI(8)=	P= 8.21649929E+04 CI= 3.12500000E-02 CII(4)= 2.29768144D-01 CII(5)= 8.36573719D-03 CII(6)= 2.74176331E-01 CII(7)= 5.32264246E-03 EVI(4)= 0. EVI(5)= 1.63123379D+10	RHO= 2.63148167E-06 SUM(CI)= 1.00011573E+00 CII(5)= 8.36573719D-03 CII(6)= 2.74176331E-01 CII(7)= 5.32264246E-03 EVI(5)= 1.63123379D+10
6	56	X= 1.20843750D+00 U= 1.67681656E+C5 CII(1)= 4.66845327D-01 CII(6)= 8.73072130D-04 CII(7)= 3.18095354E-01 CII(8)= 5.5398939E-04 CII(9)= 1.60724407D+10 EVI(6)= 1.49719903D+10 EVI(7)= 0.	H= 2.31567803D+11 T= 6.9746691E+03 CII(2)= 1.38760385D-04 CII(7)= 1.59619609D-08 CII(8)= 8.27762899E-05 CII(9)= 5.5398939E-04 EVI(2)= 1.53273478D+10 EVI(7)= 0.	MU= 1.90393191E+01 E= 2.01188398E+11 CII(3)= 2.94410136D-01 CII(8)= 4.01205672E-01 CII(9)= 0. EVI(3)= 0. EVI(8)=	P= 7.45361547E+04 CI= 3.12500000E-02 CII(4)= 2.30188969D-01 CII(5)= 7.66083040D-03 CII(6)= 2.74632032E-01 CII(7)= 4.87336832E-03 EVI(4)= 0. EVI(5)= 1.57786668D+10	RHO= 2.45350937E-06 SUM(CI)= 1.00011511E+00 CII(5)= 7.66083040D-03 CII(6)= 2.74632032E-01 CII(7)= 4.87336832E-03 EVI(5)= 1.57786668D+10
6	61	X= 1.36466750D+00 U= 1.85845941E+05 CII(1)= 4.67367106D-01 CII(6)= 8.28998908D-04 CII(7)= 3.18421756E-01 CII(8)= 5.27311966E-04 CII(9)= 1.54695925D+10 EVI(6)= 1.44693551D+10 EVI(7)= 0.	H= 2.28357015D+11 T= 6.76738218E+03 CII(2)= 1.20563349D-04 CII(7)= 1.51561377D-08 CII(8)= 7.19144303E-05 CII(9)= 5.27311966E-04 EVI(2)= 1.79363920D+10 EVI(7)= 0.	MU= 1.90875734E+01 E= 1.98677791E+11 CII(3)= 2.94229007D-01 CII(8)= 4.00922170E-01 CII(9)= 0. EVI(3)= 0. EVI(8)=	P= 6.70211678E+04 CI= 3.12500000E-02 CII(4)= 2.30594218D-01 CII(5)= 6.97516501D-03 CII(6)= 2.75092753E-01 CII(7)= 4.43678265E-03 EVI(4)= 0. EVI(5)= 1.52118590D+10	RHO= 2.27350516E-06 SUM(CI)= 1.00011507E+00 CII(5)= 6.97516501D-03 CII(6)= 2.75092753E-01 CII(7)= 4.43678265E-03 EVI(5)= 1.52118590D+10

CHECK,ABS((HPREV-H)/H).GT.HCHECKT

REDUCED SPEC= 6.25000000E-02 IPSI,IX=

IFEXP,ITNEG= 0 0

6 66 X= 1.70843750D+00
U= 2.12511171E+C5
CII(1)= 4.68501300D-01
CII(6)= 7.40553177D-04
CII(7)= 3.19166022E-01
CII(8)= 4.71011108E-04
CII(9)= 1.4476C531D+10
EVI(6)= 1.34821171D+10
EVI(7)= 0.

H= 2.23045873D+11
T= 6.42516536E+03
CII(2)= 8.86116550D-05
CII(7)= 1.35391324D-08
CII(8)= 5.28509769E-05
CII(9)= 4.71011108E-04
EVI(2)= 1.39132112D+10
EVI(7)= 0.

MU= 1.90856695E+01
E= 1.950544873E+11
CII(3)= 2.93754933D-01
CII(8)= 4.00240457E-01
CII(9)= 0.
EVI(3)= 0.
EVI(8)=

P= 5.66814721E+04
CI= 6.25000000E-02
CII(4)= 2.31380260D-01
CII(5)= 5.64883609D-03
CII(6)= 2.76005841E-01
CII(7)= 3.59280687E-03
EVI(4)= 0.
EVI(5)= 1.42771529D+10

RHO= 2.02498915E-06
SUM(CI)= 1.00011454E+00
CII(5)= 5.64883609D-03
CII(6)= 2.76005841E-01
CII(7)= 3.59280687E-03
EVI(5)= 1.42771529D+10

APPENDIX A - Continued

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
 REDUCED SPEC= 6.2500000E-02 IPSI,IX= 6 69 T,PREV,H,HPREV= 5.9795305E+03 6.2402299E+03 2.1642890E+11 2.2029817E+11
 IEXP,ITNEG= 0 0
 6 71
 X= 2.145937500+CC
 U= 2.41664672E+05
 CII(1)= 4.6967583E-01 CII(2)= 6.0662392E-05 CII(3)= 1.9031585E+11 MU= 1.98851824E+01 P= 4.44641349E+04 RHO= 1.70297964E-06
 CII(6)= 6.493753500-04 CII(7)= 1.18722507D-08 CII(8)= 2.92223849D-01 CII(4)= 2.32143172D-01 CII(5)= 4.36283422D-03
 CM(1)= 3.19954633E-01 CM(2)= 3.61797759E-05 CM(3)= 3.9502473E-01 CM(4)= 2.76905924E-01 CM(5)= 2.77477629E-03
 CM(6)= 4.13007309E-04 CM(7)= 4.13007309E-04 CM(8)= 3.9502473E-01 CM(4)= 2.76905924E-01 CM(5)= 2.77477629E-03
 EVI(1)= 1.32251782D+10 EVI(2)= 1.28030174D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 1.30991912D+10
 EVI(6)= 1.23147724D+10 EVI(7)= 0. EVI(8)=

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
 REDUCED SPEC= 6.2500000E-02 IPSI,IX= 6 72 T,PREV,H,HPREV= 5.7033703E+03 5.9856968E+03 2.1228651E+11 2.1642547E+11
 IEXP,ITNEG= 0 0
 6 75
 X= 2.458437500+CC
 U= 2.62412947E+05
 CII(1)= 4.7038435E-01 CII(2)= 4.56979778D-05 CII(3)= 1.86602696E+11 MU= 1.98850612E+01 P= 3.62363458E+04 RHO= 1.47341756E-06
 CII(6)= 5.9355C5500-04 CII(7)= 1.08515630D-08 CII(8)= 2.92892966D-01 CII(4)= 2.32589561D-01 CII(5)= 3.61119871D-03
 CM(1)= 3.20435278E-01 CM(2)= 2.72546470E-05 CM(3)= 3.95049127E-01 CM(4)= 2.77436625E-01 CM(5)= 2.29671916E-03
 CM(6)= 3.77457620E-04 CM(7)= 3.77457620E-04 CM(8)= 3.95049127E-01 CM(4)= 2.77436625E-01 CM(5)= 2.29671916E-03
 EVI(1)= 1.22205778D+10 EVI(2)= 1.19130794D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 1.21524022D+10
 EVI(6)= 1.13776846D+10 EVI(7)= 0. EVI(8)=

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6 1
 X= 6.00000000D-C2
 U= 1.9564560E+04
 CII(1)= 7.68000000D-C1 CII(2)= 2.32000000D-01 CII(3)= 0. MU= 2.88492827E+01 P= 1.17957231E+05 RHO= 2.32581613E-06
 CII(6)= 0. CII(7)= 0. CII(8)= 0. CII(4)= 0. CII(5)= 0.
 CM(1)= 7.90842701E-01 CM(2)= 2.09157299E-01 CM(3)= 0. CM(4)= 0. CM(5)= 0.
 CM(6)= 0. CM(7)= 0. CM(8)= 0. EVI(1)= 4.73529195D+10 EVI(2)= 4.28310041D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 4.50619000D+10
 EVI(6)= 4.41721177D+10 EVI(7)= 0. EVI(8)=

-----CHECKT= 1.04575000E+02

6 6
 X= 1.38125000D-01
 U= 3.12138764E+04
 CII(1)= 5.74472092D-01 CII(2)= 2.46577501D-03 CII(3)= 1.70295317D-01 MU= 2.10884979E+01 P= 1.17241755E+05 RHO= 2.71857690E-06
 CII(6)= 9.28312177D-04 CII(7)= 1.69718284D-08 CII(8)= 2.92223849D-01 CII(4)= 2.09782081D-01 CII(5)= 4.13588691D-02
 CM(1)= 4.32422669E-01 CM(2)= 1.62458673E-05 CM(3)= 2.59082791E-01 CM(4)= 2.76499310E-01 CM(5)= 2.90654774E-02
 CM(6)= 6.52383011E-04 CM(7)= 6.52383011E-04 CM(8)= 2.59082791E-01 CM(4)= 2.76499310E-01 CM(5)= 2.90654774E-02
 EVI(1)= 2.76846690D+10 EVI(2)= 2.55675736D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.66710023D+10
 EVI(6)= 2.58146601D+10 EVI(7)= 0. EVI(8)=

6 7
 X= 1.53750000E-01
 U= 3.35263367E+04
 CII(1)= 5.64268901D-01 CII(2)= 2.04233466D-03 CII(3)= 1.83463532D-01 MU= 2.08832587E+01 P= 1.17011006E+05 RHO= 2.76444488E-06
 CII(6)= 1.68385310D-03 CII(7)= 1.98154987D-08 CII(8)= 2.92223849D-01 CII(4)= 2.11538758D-01 CII(5)= 3.87105716D-02
 CM(1)= 4.20608704E-01 CM(2)= 1.33283134E-03 CM(3)= 2.73509166E-01 CM(4)= 2.76101163E-01 CM(5)= 2.65395788E-02
 CM(6)= 7.54278346E-04 CM(7)= 7.54278346E-04 CM(8)= 2.73509166E-01 CM(4)= 2.76101163E-01 CM(5)= 2.65395788E-02
 EVI(1)= 2.67843977D+10 EVI(2)= 2.47724633D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.58245220D+10
 EVI(6)= 2.49706609D+10 EVI(7)= 0. EVI(8)=

CHECK, ABSI (MPREV-HI/HI), GT, HC CHECK REDUCED SPEC= 6.25000000E-02 IPSI, IX= IEXP, ITNEG= 0	6	31	T, IPREV, H, HPREV =	7.1125002E+03	7.3719752E+03	2.1903267E+11	2.2287013E+11
6 32	X= 1.66937500D+0C U= 2.20978519D+11 H= 2.20978519D+11 T= 7.259343407E+03		MU= 1.96526627E+01 E= 1.90290937E+11		P= 5.78340282E+04 CI= 6.25070000E-02 SUM(CI)= 1.0C113714E+33	RHO= 1.88458232E-06	
	CI(1)= 5.06267563D-01 CI(6)= 9.78459608D-04 CI(1)= 3.55138095E-01 CI(6)= 3.9521042E-04	CI(2)= 2.88697733D-04 CI(7)= 1.78527480D-08 CI(8)= 1.77302474E-04 CI(9)= 6.39521042E-04	CI(3)= 3.556585597E-01 CI(4)= 2.79193868E-01 CI(5)= 8.22609615E-03		CI(4)= 2.27302629D-01 CI(5)= 1.25605724D-02		
	EVII(1)= 1.68842637D+10 EVII(6)= 1.57296782D+10	EVII(2)= 1.60455292D+10 EVII(7)= 0.	EVII(3)= 0. EVII(4)= 0. EVII(5)= 1.65416013D+10				

APPENDIX A - Continued

CHECK,ABS((H/REV-H)/H).GT.HCHECKT
 REDUCED SPEC= 6.2500000E-02 IPSI,IX= 6 34 T,TPREV,H,MPREV= 6.8461061E+03 7.1190266E+03 2.1494755E+11 2.1902952E+11
 IEXP,ITNEG= 0 0
 CHECK,ABS((H/REV-H)/H).GT.HCHECKT
 REDUCED SPEC= 6.2500000E-02 IPSI,IX= 6 37 T,TPREV,H,MPREV= 6.5604525E+03 6.8530523E+03 2.1058484E+11 2.1494386E+11
 IEXP,ITNEG= 0 0
 H= 2.13879677D+11 MU= 1.9647068E+01 P= 4.55395998E+04 RHO= 1.58437232E-06
 T= 6.79182707E+03 E= 1.85136490E+11 CI= 3)= 2.5314141D-01 CI(4)= 2.28560537D-01 CI(5)= 1.04455632D-02
 CI(1)= 2.1859643D-04 CI(7)= 1.58663202D-08 CM(2)= 1.34211846E-01 CM(3)= 3.55046164E-01 CM(4)= 2.80659034E-01 CM(5)= 6.83899950E-03
 CM(1)= 8.6784393D-04 CM(8)= 5.68201455E-04 CM(6)= 1.55406462D+10 EVI(2)= 1.48565627D+10 EVI(3)= 0.
 EVI(4)= 0. EVI(5)= 1.52786777D+10
 EVI(6)= 1.44736686D+10 EVI(7)= 0.

CHECK,ABS((H/REV-H)/H).GT.HCHECKT
 REDUCED SPEC= 3.12500000E-02 IPSI,IX= 6 39 T,TPREV,H,MPREV= 6.5679443E+03 6.7172012E+03 2.1058064E+11 2.1279894E+11
 IEXP,ITNEG= 0 0
 CHECK,ABS((H/REV-H)/H).GT.HCHECKT
 REDUCED SPEC= 3.12500000E-02 IPSI,IX= 6 42 T,TPREV,H,MPREV= 6.4165746E+03 6.5721089E+03 2.0827823E+11 2.1057945E+11
 IEXP,ITNEG= 0 0
 H= 2.10011570D+11 MU= 1.56459598E+01 P= 3.97042701E+04 RHO= 1.43463647E-06
 T= 6.53916866E+03 E= 1.82336078E+11 CI= 3)= 2.52782115D-01 CI(4)= 2.29113219D-01 CI(5)= 9.51299515D-03
 CI(1)= 5.0872434D-01 CI(7)= 1.49898092D-08 CM(2)= 1.16101508E-01 CM(3)= 3.54522221E-01 CM(4)= 2.81321818E-01 CM(5)= 6.22806986E-03
 CM(1)= 8.19901194D-04 CM(8)= 5.36781722E-04 CM(6)= 1.48007791D+10 EVI(2)= 1.42064084D+10 EVI(3)= 0.
 CM(1)= 3.56738225E-01 CM(7)= 5.36781722E-04 CM(8)= 5.36781722E-04 EVI(4)= 0. EVI(5)= 1.45883774D+10
 EVI(6)= 1.37907689D+10 EVI(7)= 0.

6 44 X= 2.41937500D+00 H= 2.08276928D+11 MU= 1.96456718E+01 P= 3.72657849E+04 RHO= 1.37029682E-06
 U= 2.73310972E+05 T= 6.42564084E+03 E= 1.81081517E+11 CI= 3)= 2.52625360D-01 CI(4)= 2.29336953D-01 CI(5)= 9.13481642D-03
 CI(1)= 5.09066752D-01 CI(7)= 1.77423419D-04 CM(2)= 1.08925071E-01 CM(3)= 3.54297181E-01 CM(4)= 2.81592408E-01 CM(5)= 5.98039208E-03
 CI(6)= 8.00395886D-04 CM(8)= 1.46330213D-08 CM(6)= 5.23957549E-04 CM(7)= 5.23957549E-04 EVI(2)= 1.39144338D+10 EVI(3)= 0.
 CM(1)= 3.56973095E-01 CM(7)= 5.23957549E-04 CM(8)= 5.23957549E-04 EVI(4)= 0. EVI(5)= 1.42784505D+10
 EVI(1)= 1.44774320D+10 EVI(6)= 1.34834039D+10 EVI(7)= 0.

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7 1 X= 1.20000000D-01 H= 2.44819957D+11 MU= 2.88492827E+01 P= 1.17670402E+05 RHO= 2.32455051E-06
 U= 3.98710378E+04 T= 1.75637484E+04 E= 1.94159245E+11 CI= 3)= 0. CI(4)= 0. CI(5)= 0.
 CI(1)= 0. CI(7)= 0. CM(2)= 2.09157299E-01 CM(3)= 0. CM(4)= 0. CM(5)= 0.
 CM(1)= 7.90842701E-01 CM(7)= 0. CM(8)= 0. EVI(2)= 4.27447765D+10 EVI(3)= 0.
 EVI(1)= 4.72565978D+10 EVI(6)= 4.40803277D+10 EVI(7)= 0.

-----CHECK= 1.32771000E+02

7 6 X= 2.76250000D-01 H= 2.43734420D+11 MU= 2.11102459E+01 P= 1.14960063E+05 RHO= 2.68217629E-06
 U= 6.15134412E+04 T= 1.08819545E+04 E= 2.00873679E+11 CI= 3)= 1.70742496D-01 CI(4)= 2.09775614D-01 CI(5)= 4.15909755D-02
 CI(1)= 5.75635622D-01 CI(7)= 1.68153571D-08 CM(2)= 1.63905498E-03 CM(3)= 2.57283830E-01 CM(4)= 2.76775926E-01 CM(5)= 2.92587217E-02
 CI(6)= 9.19733629D-04 CM(8)= 6.47034968E-04 CM(6)= 6.47034968E-04 CM(7)= 6.47034968E-04

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CHECK,ABS((HPREV-H)/H).GT.HCHECKT

9 25 X= 1.3650000000000000

9 26

9 27

9 28

APPENDIX A - Continued

9	29	X= 1.615000000+00 U= 2.590131713E+05 CII(1)= 5.490168180-01 CII(6)= 1.177278360-03 CII(11)= 4.00522436E-01 CII(16)= 8.01843177E-04 EVI(1)= 1.968527610+10 EVI(6)= 1.834403610+10	H= 2.170625950+11 T= 8.21251309E+03 CII(2)= 8.811206260-04 CII(7)= 2.152354210-08 CII(12)= 5.62727307E-04 CII(17)= 8.01843177E-04 EVI(2)= 1.851957850+10 EVI(7)= 0.	MU= 2.04384204E+01 E= 1.83652723E+11 CII(3)= 2.050765940-01 CII(8)= 2.99217708E-01 CII(13)= 2.99217708E-01 CII(18)= 0.	P= 5.98147054E+04 CI= 6.25000000E-02 CII(4)= 2.196945820-01 CII(9)= 2.80638139E-01 CII(14)= 2.80638139E-01 EVI(4)= 0. EVI(9)= 1.917132670+10	RHO= 1.79033029E-06 SUM(CI)= 1.00147449E+00 CI(5)= 2.562807610-02 CM(5)= 1.74552584E-02
9	30	X= 1.677500000+00 U= 2.43310119E+05 CII(1)= 5.49085350-01 CII(6)= 1.162232710-03 CII(11)= 4.00442906E-01 CII(16)= 7.91346577E-04 EVI(1)= 1.946712080+10 EVI(6)= 1.814034120+10	H= 2.160264650+11 T= 8.13794587E+03 CII(2)= 8.526407880-04 CII(7)= 2.124847080-08 CII(12)= 5.44538585E-04 CII(17)= 7.91346577E-04 EVI(2)= 1.832707300+10 EVI(7)= 0.	MU= 2.04319908E+01 E= 1.82909527E+11 CII(3)= 2.052550530-01 CII(8)= 2.99383892E-01 CII(13)= 2.99383892E-01 CII(18)= 0.	P= 5.79791940E+04 CI= 6.25000000E-02 CII(4)= 2.199995520-01 CII(9)= 2.80939301E-01 CII(14)= 2.80939301E-01 EVI(4)= 0. EVI(9)= 1.896663590+10	RHO= 1.75074139E-06 SUM(CI)= 1.00147442E+00 CI(5)= 2.512417550-02 CM(5)= 1.71066689E-02
9	31	X= 1.740000000+00 U= 2.47592048E+05 CII(1)= 5.491751780-01 CII(6)= 1.147189070-03 CII(11)= 4.00404559E-01 CII(16)= 7.80888584E-04 EVI(1)= 1.924526690+10 EVI(6)= 1.793707060+10	H= 2.149754610+11 T= 8.06346199E+03 CII(2)= 8.260617820-04 CII(7)= 2.097343600-08 CII(12)= 5.27295026E-04 CII(17)= 7.80888584E-04 EVI(2)= 1.813480560+10 EVI(7)= 0.	MU= 2.04263667E+01 E= 1.82152596E+11 CII(3)= 2.053898170-01 CII(8)= 2.99497981E-01 CII(13)= 2.99497981E-01 CII(18)= 0.	P= 5.61590281E+04 CI= 6.25000000E-02 CII(4)= 2.202929770-01 CII(9)= 2.81236571E-01 CII(14)= 2.81236571E-01 EVI(4)= 0. EVI(9)= 1.8762202920+10	RHO= 1.71097279E-06 SUM(CI)= 1.00147435E+00 CI(5)= 2.463910950-02 CM(5)= 1.67717770E-02
9	32	X= 1.802500000+00 U= 2.51861769E+05 CII(1)= 5.493080120-01 CII(6)= 1.132185580-03 CII(11)= 4.00402792E-01 CII(16)= 7.70490394E-04 EVI(1)= 1.903123590+10 EVI(6)= 1.773356460+10	H= 2.139051970+11 T= 7.98889727E+03 CII(2)= 8.005584750-04 CII(7)= 2.069913530-08 CII(12)= 5.10892752E-04 CII(17)= 7.70490394E-04 EVI(2)= 1.794235300+10 EVI(7)= 0.	MU= 2.04214542E+01 E= 1.81382030E+11 CII(3)= 2.054858210-01 CII(8)= 2.95565908E-01 CII(13)= 2.95565908E-01 CII(18)= 0.	P= 5.43555370E+04 CI= 6.25000000E-02 CII(4)= 2.205762620-01 CII(9)= 2.81530499E-01 CII(14)= 2.81530499E-01 EVI(4)= 0. EVI(9)= 1.855759700+10	RHO= 1.67108120E-06 SUM(CI)= 1.00147429E+00 CI(5)= 2.417062920-02 CM(5)= 1.64489267E-02
9	33	X= 1.865000000+00 U= 2.56121711E+05 CII(1)= 5.494658600-01 CII(6)= 1.117268140-03 CII(11)= 4.00433213E-01 CII(16)= 7.60179004E-04 EVI(1)= 1.881258600+10 EVI(6)= 1.752948200+10	H= 2.128272070+11 T= 7.91409998E+03 CII(2)= 7.761551160-04 CII(7)= 2.042640780-08 CII(12)= 4.95217852E-04 CII(17)= 7.60179004E-04 EVI(2)= 1.774932460+10 EVI(7)= 0.	MU= 2.04171682E+01 E= 1.80597817E+11 CII(3)= 2.055475670-01 CII(8)= 2.95593036E-01 CII(13)= 2.95593036E-01 CII(18)= 0.	P= 5.25686899E+04 CI= 6.25000000E-02 CII(4)= 2.208505680-01 CII(9)= 2.81821450E-01 CII(14)= 2.81821450E-01 EVI(4)= 0. EVI(9)= 1.835238400+10	RHO= 1.63107927E-06 SUM(CI)= 1.00147429E+00 CI(5)= 2.371684840-02 CM(5)= 1.61367250E-02
		CII(6)= 4.741931660-04 CII(11)= 4.81604662E-01 CII(16)= 3.46758629E-04 EVI(1)= 2.96645300+10 EVI(6)= 2.765926850+10	CII(7)= 8.669416640-09 CII(12)= 4.3711114E-03 CII(17)= 3.46758629E-04 EVI(2)= 2.730482950+10 EVI(7)= 0.	CII(8)= 2.01365292E-01 CII(13)= 2.95593036E-01 CII(18)= 0.	CII(4)= 2.74574484E-01 CII(9)= 2.81821450E-01 CII(14)= 2.81821450E-01 EVI(4)= 0. EVI(9)= 1.835238400+10	CM(5)= 3.72848535E-02 CM(5)= 1.61367250E-02 CM(5)= 2.852075720+10

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10 6

10	7	X= 6.7500C000D-C1 U= 1.47256742E+C5 C1(1)= 5.91568594D-01 C1(6)= 7.53982282D-C4 C1(6)= 4.52172228E-01 CM(6)= 5.38336641E-04 EVI(1)= 2.7156C892D+1C EVI(6)= 2.53176291D+1C	H= 2.34778207D+11 T= 1.67572C92E+C4 C1(2)= 3.07129244D-03 C1(7)= 1.37856494E+C8 CM(2)= 2.05636829E-03 CM(7)= 2.38336641E-04 EVI(2)= 2.50593822D+1C EVI(7)= 0.	MU= 2.14254379E+C1 E= 1.930321E+11 C1(3)= 1.53918609D-01 C1(8)= 1.235426731E-01 CM(3)= 2.53836641E-04 CM(8)= 2.38336641E-04 EVI(3)= C. EVI(8)= C.	P= 1.61830197E+C5 CI= 6.25000300E-C2 C1(4)= 2.66436C56D-01 CM(4)= 2.766428932E-01 CM(5)= 3.23C570482E-C2	RHO= 2.43927415E-C6 SUM(C1)= 1.0C138869E+C0 C1(5)= 4.52457444D-C2
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LELE2= 1.C000000E+00 1.3000000E+00 1.0000000E+00 1.0000000E+00

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MAXL= 16  
PST= 6.0000000E-02 1.2000000E-01 1.8000000E-01 2.4000000E-01 3.0000000E-01  
3.6000000E-01 4.2000000E-01 4.8000000E-01 5.4000000E-01 6.0000000E-01  
6.6000000E-01 7.2000000E-01 7.8000000E-01 8.4000000E-01 9.0000000E-01
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9	25	X=	H=	MU=	P=	RHO=
U=	2.0695744E+05	2.21273066D+11	2.04766711E+01	6.75445715E+04	1.95011368E-06	
C1(1)=	5.4921192D+03	T= 1.01769129E-03	E= 1.8663684E+11	C1= 6.2500000E-02	SUM(C1)= 1.00147459E+00	
C1(6)=	1.23621240D+03	C1(7)= 2.26010013D+08	C1(8)= 2.03797815D-01	C1(4)= 2.183202198D-01	C1(5)= 2.78907317D-02	
C1(1)=	4.01375409E-01	CM(2)= 6.51152953E-04	CM(3)= 2.97879300E-01	CM(4)= 2.79377141E-01	CM(5)= 1.903006439E-02	
CM(6)=	8.43476485E-04	CM(7)= 8.43476485E-04	CM(8)= 2.97879300E-01	CM(4)= 2.79377141E-01	CM(5)= 1.903006439E-02	
EV1(1)=	1.52019326D+10	EV1(2)= 1.93370408D+10	EV1(3)= 0.	EV1(4)= 0.	EV1(5)= 2.006406481D+10	
EV1(6)=	1.50209332D+10	EV1(7)= 0.	EV1(8)=			

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9 30
X = 1.6775000CD+00
U = 2.43310119E+05
C( 1) = 5.49080535D-01
C( 6) = 1.36223710-03
H = 2.16026465D+11
T = 8.13794587E+03
I( 2) = 8.52840768D-04
C( 7) = 2.12484708D-08
MU = 2.04319908E+01
E = 1.82909527E+11
C( 3) = 2.05255063D-01
C( 8) = 2.19999552D-01
P = 5.79791940E+04
CI = 6.25000000E-02
SUM(CI) = 1.0017442E+00
RHO = 1.75074139E-06

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APPENDIX A - Continued

CM(1)= 4.C0442906E-01 CM(2)= 5.44538585E-04 CM(3)= 2.99383892E-01 CM(4)= 2.80939301E-01 CM(5)= 1.71066689E-02
CM(6)= 7.51346577E-04 CM(7)= 7.91346577E-04 CM(8)=
EVI(1)= 1.54671208D+10 EVI(2)= 1.83270730D+10 EVI(3)= 0.
EVI(4)= 0.
EVI(5)= 1.89666359D+10
EVI(6)= 1.81404122D+10 EVI(7)= 0.

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
REDUCED SPEC= 3.12500000E-02 IPSI,IX= 9 34 T,TPREV,H,HPREV= 7.7530198E+03 7.9088102E+03 2.1061436E+11 2.1282721E+11
IEXP,ITNEG= 0 0
X= 1.52750000D+00 MU= 2.04134152E+01
U= 6.0376595E+05 E= 1.79800848E+11 RHO= 1.59107015E-06
CII(1)= 5.49644025D-01 CII(2)= 7.52970571D-04 CII(3)= 2.05581032D-01 CII(4)= 2.21115546D-01 CII(5)= 2.32787274D-02
CII(6)= 1.10256334D-03 CII(7)= 2.01575680D-08 CII(8)=
CM(1)= 4.C0489424E-01 CM(2)= 4.80334403E-04 CM(3)= 2.99586734E-01 CM(4)= 2.82107715E-01 CM(5)= 1.58357214E-02
CM(6)= 7.50036098E-04 CM(7)= 7.50036098E-04 CM(8)=
EVI(1)= 1.65917636D+10 EVI(2)= 1.75543470D+10 EVI(3)= 0.
EVI(4)= 0.
EVI(5)= 1.81451111D+10
EVI(6)= 1.73233725D+10 EVI(7)= 0.

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
REDUCED SPEC= 3.12500000E-02 IPSI,IX= 9 37 T,TPREV,H,HPREV= 7.5992688E+03 7.7577726E+03 2.0833031E+11 2.1061323E+11
IEXP,ITNEG= 0 0
X= 1.46250000D+00 MU= 2.04038315E+01 RHO= 1.45045777E-06
U= 7.75247469E+05 E= 1.76896846E+11
CII(1)= 5.56423249D-01 CII(2)= 6.77463993D-04 CII(3)= 2.05503778D-01 CII(4)= 2.21992953D-01 CII(5)= 2.182564438D-02
CII(6)= 1.03188641D-03 CII(7)= 1.92310691D-08 CII(8)=
CM(1)= 4.C0868904E-01 CM(2)= 4.31944411E-04 CM(3)= 2.99333556E-01 CM(4)= 2.83094176E-01 CM(5)= 1.48409478E-02
CM(6)= 7.15226374E-04 CM(7)= 7.15226374E-04 CM(8)=
EVI(1)= 1.78080548D+10 EVI(2)= 1.68620967D+10 EVI(3)= 0.
EVI(4)= 0.
EVI(5)= 1.74093113D+10
EVI(6)= 1.65918894D+10 EVI(7)= 0.

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
REDUCED SPEC= 3.12500000E-02 IPSI,IX= 9 43 T,TPREV,H,HPREV= 7.2790446E+03 7.4465641E+03 2.0352114E+11 2.0596715E+11
IEXP,ITNEG= 0 0
X= 2.36500000D+00 MU= 2.03981991E+01 RHO= 1.30961012E-06
U= 2.90195609E+05 E= 1.73804276E+11
CII(1)= 5.51359847D-01 CII(2)= 6.09421406D-04 CII(3)= 2.05217759D-01 CII(4)= 2.22804137D-01 CII(5)= 2.04821723D-02
CII(6)= 1.00314447D-03 CII(7)= 1.83399467D-08 CII(8)=
CM(1)= 4.C1440174E-01 CM(2)= 3.88471849E-04 CM(3)= 2.98834430E-01 CM(4)= 2.84950196E-01 CM(5)= 1.39229348E-02
CM(6)= 6.81896183E-04 CM(7)= 6.81896183E-04 CM(8)=
EVI(1)= 1.69907942D+10 EVI(2)= 1.61397294D+10 EVI(3)= 0.
EVI(4)= 0.
EVI(5)= 1.66416879D+10
EVI(6)= 1.58291062D+10 EVI(7)= 0.

CHECK,ABS((HPREV-H)/H).GT.HCHECKT
REDUCED SPEC= 3.12500000E-02 IPSI,IX= 9 46 T,TPREV,H,HPREV= 7.1103954E+03 7.2840460E+03 2.0097722E+11 2.0351963E+11
IEXP,ITNEG= 0 0
X= 2.42750000D+00 MU= 2.03970875E+01 RHO= 1.26920372E-06
U= 2.94503464E+05 E= 1.72884239E+11
CII(1)= 5.51642549D-01 CII(2)= 5.91295586D-04 CII(3)= 2.05111930D-01 CII(4)= 2.23024331D-01 CII(5)= 2.04821723D-02
CII(6)= 9.89715308D-04 CII(7)= 1.80944286D-08 CII(8)=
CM(1)= 4.C1624420E-01 CM(2)= 3.76897119E-04 CM(3)= 2.98664049E-01 CM(4)= 2.84315425E-01 CM(5)= 1.36740471E-02
CM(6)= 6.72730930E-04 CM(7)= 6.72730930E-04 CM(8)=
EVI(1)= 1.67470237D+10 EVI(2)= 1.59241599D+10 EVI(3)= 0.
EVI(4)= 0.
EVI(5)= 1.64126535D+10
EVI(6)= 1.56015885D+10 EVI(7)= 0.

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10 1 X= 3.000000000-01 H= 2.404869070+11 MU= 2.88492827E+01 P= 1.15519835E+05 RHO= 2.31503169E-06
 U= 5.85980337E+04 T= 1.73136478E+04 E= 1.90587014E+11 CI= 6.25000000E-02 SUM(CI)= 1.00000000E+00
 CI(1)= 7.68000000-01 CI(2)= 2.32000000-01 CI(3)= 0. CI(4)= 0. CI(5)= 0.

CHECK= 2.6C5850C0E+02

CHECK,ABS((HPREV-H)/H).GT.HCHECK

REDUCED SPEC= 3.12500000E-02 IPSI,IX= 43 3 T,IPREV,H,HPREV= 9.1125061E+03 9.4064075E+03 1.1877390E+11 1.2096168E+11

IEXP,ITNEG= 0 0

43 4 X= 2.405000000+00 H= 1.19867536D+11 MU= 2.85908929E+01 P= 5.30244443E+04 RHO= 1.96285869E-06

U= 5.01515375E+05 T= 9.28899537E+03 E= 9.28536448E+10 CI= 3.12500000E-02 SUM(CI)= 1.00000144E+00

CI(1)= 7.676221270-01 CI(2)= 2.22006662D-01 CI(3)= 2.90116448D-04 CI(4)= 9.69147933D-03 CI(5)= 1.91055390D-04

CI(6)= 1.44313645D-09 CI(7)= 2.63840822D-14 CI(8)= 5.92139435E-04 CM(3)= 5.92139435E-04 CM(4)= 1.73180030E-02 CM(5)= 1.82032930E-04

CM(1)= 7.83373857E-01 CM(2)= 1.98533965E-09 CM(3)= 1.37498536E-09 CM(4)= 1.73180030E-02 CM(5)= 1.82032930E-04

CM(6)= 1.37498536E-09 CM(7)= 2.13008860D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.21297464D+10

EVI(1)= 2.28402441D+10 EVI(2)= 2.13008860D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.21297464D+10

EVI(6)= 2.12889391D+10 EVI(7)= 0. EVI(8)=

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44 1 X= 2.340000000+00 H= 1.19006670D+11 MU= 2.88492827E+01 P= 5.59680556E+04 RHO= 2.07651949E-06
 U= 4.80169891E+05 T= 9.35175595E+03 E= 9.20538501E+10 CI= 6.25000000E-02 SUM(CI)= 1.00000000E+00
 CI(1)= 7.68000000-01 CI(2)= 2.32000000-01 CI(3)= 0. CI(4)= 0. CI(5)= 0.

CI(6)= 0. CI(7)= 0. CI(8)= 0. CM(3)= 0. CM(4)= 0. CM(5)= 0.

CM(1)= 7.50842701E-01 CM(2)= 2.09157299E-01 CM(3)= 0. CM(4)= 0. CM(5)= 0.

CM(6)= 0. CM(7)= 0. CM(8)= 0. EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.23023988D+10

EVI(1)= 2.30244647D+10 EVI(2)= 2.14631521D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.23023988D+10

EVI(6)= 2.14608984D+10 EVI(7)= 0. EVI(8)=

CHECK= 2.61445000E+02

CHECK,ABS((HPREV-H)/H).GT.HCHECK

REDUCED SPEC= 3.12500000E-02 IPSI,IX= 43 3 T,IPREV,H,HPREV= 9.1125061E+03 9.4064075E+03 1.1877390E+11 1.2096168E+11

IEXP,ITNEG= 0 0

44 2 X= 2.402500000+00 H= 1.24233577D+11 MU= 2.87044863E+01 P= 5.37622913E+04 RHO= 1.92366587E-06

U= 4.52728308E+05 T= 9.64832328E+03 E= 9.62879467E+10 CI= 6.25000000E-02 SUM(CI)= 1.00000673E+00

CI(1)= 7.6779894D-01 CI(2)= 2.26587886D-01 CI(3)= 1.76680344D-04 CI(4)= 5.38645261D-03 CI(5)= 5.67742969D-05

CI(6)= 2.53988286D-10 CI(7)= 4.64353018D-15 CI(8)= 3.62044439E-04 CM(3)= 3.62044439E-04 CM(4)= 5.66345969E-03 CM(5)= 5.43080854E-05

CM(1)= 7.66667410E-01 CM(2)= 2.03252777E-01 CM(3)= 3.62044439E-04 CM(4)= 5.66345969E-03 CM(5)= 5.43080854E-05

CM(6)= 2.42955321E-10 CM(7)= 2.42955321E-10 CM(8)= 0. EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.31184647D+10

EVI(1)= 2.38993336D+10 EVI(2)= 2.22300621D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.31184647D+10

EVI(6)= 2.22738097D+10 EVI(7)= 0. EVI(8)=

CHECK= 2.61679C0E+02

CHECK,ABS((HPREV-H)/H).GT.HCHECK

REDUCED SPEC= 3.12500000E-02 IPSI,IX= 43 3 T,IPREV,H,HPREV= 9.1125061E+03 9.4064075E+03 1.1877390E+11 1.2096168E+11

IEXP,ITNEG= 0 0

44 2 X= 2.402500000+00 H= 1.24233577D+11 MU= 2.87044863E+01 P= 5.37622913E+04 RHO= 1.92366587E-06

U= 4.52728308E+05 T= 9.64832328E+03 E= 9.62879467E+10 CI= 6.25000000E-02 SUM(CI)= 1.00000673E+00

CI(1)= 7.6779894D-01 CI(2)= 2.26587886D-01 CI(3)= 1.76680344D-04 CI(4)= 5.38645261D-03 CI(5)= 5.67742969D-05

CI(6)= 2.53988286D-10 CI(7)= 4.64353018D-15 CI(8)= 3.62044439E-04 CM(3)= 3.62044439E-04 CM(4)= 5.66345969E-03 CM(5)= 5.43080854E-05

CM(1)= 7.66667410E-01 CM(2)= 2.03252777E-01 CM(3)= 3.62044439E-04 CM(4)= 5.66345969E-03 CM(5)= 5.43080854E-05

CM(6)= 2.42955321E-10 CM(7)= 2.42955321E-10 CM(8)= 0. EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.31184647D+10

EVI(1)= 2.38993336D+10 EVI(2)= 2.22300621D+10 EVI(3)= 0. EVI(4)= 0. EVI(5)= 2.31184647D+10

EVI(6)= 2.22738097D+10 EVI(7)= 0. EVI(8)=

CHECK= 2.61679C0E+02

CHECK,ABS((HPREV-H)/H).GT.HCHECK

REDUCED SPEC= 3.12500000E-02 IPSI,IX= 43 3 T,IPREV,H,HPREV= 9.1125061E+03 9.4064075E+03 1.1877390E+11 1.2096168E+11

IEXP,ITNEG= 0 0

BEGIN PHYSICAL SPACE CALCULATIONS KSTAG= 119

X= 6.00000000E-02 R= 5.40347303E-02 Y= 2.0937752E-01 PSI= 0.
 X= 6.00000000E-02 R= 5.59869210E-02 Y= 0. PSI= 3.41887158E-04

X= 1.20000000E-01 R= 1.11148742E-01 Y= 1.54642164E-01 PSI= 0.
 X= 1.20000000E-01 R= 1.14179899E-01 Y= 1.01273230E-01 PSI= 3.41887158E-04
 X= 1.20000000E-01 R= 1.20144291E-01 Y= -3.74036088E-03 PSI= 1.36659155E-03

X= 1.80000000E-01 R= 1.66786066E-01 Y= 1.51734903E-01 PSI= 0.
 X= 1.80000000E-01 R= 1.68817364E-01 Y= 1.27798455E-01 PSI= 3.41887158E-04
 X= 1.80000000E-01 R= 1.73346952E-01 Y= 7.44225959E-02 PSI= 1.36659155E-03
 X= 1.80000000E-01 R= 1.79714188E-01 Y= -6.07767611E-04 PSI= 3.06679722E-03

APPENDIX A - Continued

X= 2.40000000E-01	R= 2.22480425E-01	Y= 1.49643037E-01	Z= 1.63296510E-01	PSI= 0.
X= 2.40000000E-01	R= 2.23970108E-01	Y= 1.36448637E-01	Z= 1.50193227E-01	PSI= 3.41887158E-04
X= 2.40000000E-01	R= 2.27608269E-01	Y= 1.04224765E-01	Z= 1.18191886E-01	PSI= 1.36659155E-03
X= 2.40000000E-01	R= 2.32926057E-01	Y= 5.71241233E-02	Z= 7.14165097E-02	PSI= 3.06679722E-03
X= 2.40000000E-01	R= 2.39431829E-01	Y= -4.98711476E-04	Z= 1.41916046E-02	PSI= 5.44413801E-03
X= 3.00000000E-01	R= 2.77602697E-01	Y= 1.50441287E-01	Z= 1.71490552E-01	PSI= 0.
X= 3.00000000E-01	R= 2.78787173E-01	Y= 1.42008033E-01	Z= 1.63146372E-01	PSI= 3.41887158E-04
X= 3.00000000E-01	R= 2.81819605E-01	Y= 1.20417639E-01	Z= 1.41784023E-01	PSI= 1.36659155E-03
X= 3.00000000E-01	R= 2.86348461E-01	Y= 8.81730372E-02	Z= 1.09879998E-01	PSI= 3.06679722E-03
X= 3.00000000E-01	R= 2.92095416E-01	Y= 4.72557704E-02	Z= 6.93949115E-02	PSI= 5.44413801E-03
X= 3.00000000E-01	R= 2.98757757E-01	Y= -1.78878533E-04	Z= 2.24612814E-02	PSI= 8.47881147E-03
X= 3.60000000E-01	R= 3.32123713E-01	Y= 1.51207882E-01	Z= 1.83801846E-01	PSI= 0.
X= 3.60000000E-01	R= 3.33102284E-01	Y= 1.45334902E-01	Z= 1.78037659E-01	PSI= 3.41887158E-04
X= 3.60000000E-01	R= 3.35692176E-01	Y= 1.29842963E-01	Z= 1.62782133E-01	PSI= 1.36659155E-03
X= 3.60000000E-01	R= 3.39649716E-01	Y= 1.06148582E-01	Z= 1.39470597E-01	PSI= 3.06679722E-03
X= 3.60000000E-01	R= 3.44741025E-01	Y= 7.56661570E-02	Z= 1.09480695E-01	PSI= 5.44413801E-03
X= 3.60000000E-01	R= 3.50769186E-01	Y= 3.95746556E-02	Z= 7.39723346E-02	PSI= 8.47881147E-03
X= 3.60000000E-01	R= 3.57401364E-01	Y= -1.33177702E-04	Z= 3.49060964E-02	PSI= 1.21346707E-02
X= 4.20000000E-01	R= 3.86611222E-01	Y= 1.51937124E-01	Z= 1.96668022E-01	PSI= 0.
X= 4.20000000E-01	R= 3.87447433E-01	Y= 1.47617759E-01	Z= 1.91842616E-01	PSI= 3.41887158E-04
X= 4.20000000E-01	R= 3.89726689E-01	Y= 1.35844483E-01	Z= 1.80325444E-01	PSI= 1.36659155E-03
X= 4.20000000E-01	R= 3.93262522E-01	Y= 1.17580483E-01	Z= 1.62458739E-01	PSI= 3.06679722E-03
X= 4.20000000E-01	R= 3.97863847E-01	Y= 9.38127901E-02	Z= 1.39208062E-01	PSI= 5.44413801E-03
X= 4.20000000E-01	R= 4.03366396E-01	Y= 6.53899148E-02	Z= 1.11403467E-01	PSI= 8.47881147E-03
X= 4.20000000E-01	R= 4.09441686E-01	Y= 3.40086019E-02	Z= 8.07047896E-02	PSI= 1.21346707E-02
X= 4.20000000E-01	R= 4.16037782E-01	Y= -6.28852922E-05	Z= 4.73744566E-02	PSI= 1.64440873E-02
X= 4.80000000E-01	R= 4.40806623E-01	Y= 1.53817099E-01	Z= 2.09445300E-01	PSI= 0.
X= 4.80000000E-01	R= 4.41546091E-01	Y= 1.50458633E-01	Z= 2.05178487E-01	PSI= 3.41887158E-04
X= 4.80000000E-01	R= 4.43606901E-01	Y= 1.41098227E-01	Z= 1.97074267E-01	PSI= 1.36659155E-03
X= 4.80000000E-01	R= 4.46836298E-01	Y= 1.26430295E-01	Z= 1.82807477E-01	PSI= 3.06679722E-03
X= 4.80000000E-01	R= 4.51073222E-01	Y= 1.07199342E-01	Z= 1.64102456E-01	PSI= 5.44413801E-03
X= 4.80000000E-01	R= 4.56162928E-01	Y= 8.40687062E-02	Z= 1.41604407E-01	PSI= 8.47881147E-03
X= 4.80000000E-01	R= 4.61857596E-01	Y= 5.82035024E-02	Z= 1.16446565E-01	PSI= 1.21346707E-02
X= 4.80000000E-01	R= 4.68030382E-01	Y= 3.01666853E-02	Z= 8.91765056E-02	PSI= 1.64440873E-02
X= 4.80000000E-01	R= 4.74681182E-01	Y= -4.12746433E-05	Z= 5.97946798E-02	PSI= 2.14070611E-02
X= 5.40000000E-01	R= 4.94677229E-01	Y= 1.56608521E-01	Z= 2.23682959E-01	PSI= 0.
X= 5.40000000E-01	R= 4.95348279E-01	Y= 1.53888841E-01	Z= 2.21052875E-01	PSI= 3.41887158E-04
X= 5.40000000E-01	R= 4.97243699E-01	Y= 1.46206942E-01	Z= 2.13624046E-01	PSI= 1.36659155E-03
X= 5.40000000E-01	R= 5.00235748E-01	Y= 1.34080545E-01	Z= 2.01897134E-01	PSI= 3.06679722E-03
X= 5.40000000E-01	R= 5.04189352E-01	Y= 1.18057086E-01	Z= 1.86401545E-01	PSI= 5.44413801E-03
X= 5.40000000E-01	R= 5.08964975E-01	Y= 9.87020918E-02	Z= 1.67684173E-01	PSI= 8.47881147E-03
X= 5.40000000E-01	R= 5.14338386E-01	Y= 7.69243343E-02	Z= 1.46623852E-01	PSI= 1.21346707E-02
X= 5.40000000E-01	R= 5.20233939E-01	Y= 5.30304041E-02	Z= 1.23517072E-01	PSI= 1.64440873E-02
X= 5.40000000E-01	R= 5.26582662E-01	Y= 2.72998330E-02	Z= 9.86341572E-02	PSI= 2.14070611E-02
X= 5.40000000E-01	R= 5.33325361E-01	Y= -2.74762121E-05	Z= 7.22071063E-02	PSI= 2.70235921E-02
X= 6.00000000E-01	R= 5.48373279E-01	Y= 1.59495847E-01	Z= 2.37981589E-01	PSI= 0.
X= 6.00000000E-01	R= 5.48991529E-01	Y= 1.57233760E-01	Z= 2.35806681E-01	PSI= 3.41887158E-04
X= 6.00000000E-01	R= 5.50743328E-01	Y= 1.50824190E-01	Z= 2.29644128E-01	PSI= 1.36659155E-03
X= 6.00000000E-01	R= 5.53528572E-01	Y= 1.40823399E-01	Z= 2.19846079E-01	PSI= 3.06679722E-03

APPENDIX A - Continued

X= 6.00000000E-01	R= 5.57248692E-01	Y= 1.27022037E-01	Z= 2.06759283E-01	PSI= 5.44413801E-03
X= 6.00000000E-01	R= 5.61755717E-01	Y= 1.10531504E-01	Z= 1.90904276E-01	PSI= 8.47881147E-03
X= 6.00000000E-01	R= 5.66849804E-01	Y= 9.18930028E-02	Z= 1.72984081E-01	PSI= 1.21346707E-02
X= 6.00000000E-01	R= 5.72460801E-01	Y= 7.13632015E-02	Z= 1.53245475E-01	PSI= 1.64440873E-02
X= 6.00000000E-01	R= 5.78566507E-01	Y= 4.90233357E-02	Z= 1.31766562E-01	PSI= 2.14070611E-02
X= 6.00000000E-01	R= 5.85118240E-01	Y= 2.50515239E-02	Z= 1.08718596E-01	PSI= 2.70235921E-02
X= 6.00000000E-01	R= 5.91970299E-01	Y= -1.91354987E-05	Z= 8.46141310E-02	PSI= 3.32936805E-02
X= 6.60000000E-01	R= 5.99096533E-01	Y= 1.62543959E-01	Z= 2.61872375E-01	PSI= 0.
X= 6.60000000E-01	R= 5.99666285E-01	Y= 1.60616444E-01	Z= 2.60035972E-01	PSI= 3.41887158E-04
X= 6.60000000E-01	R= 6.01289080E-01	Y= 1.55126443E-01	Z= 2.54805480E-01	PSI= 1.36659155E-03
X= 6.60000000E-01	R= 6.03884343E-01	Y= 1.46346516E-01	Z= 2.46440572E-01	PSI= 3.06679722E-03
X= 6.60000000E-01	R= 6.07367644E-01	Y= 1.34562306E-01	Z= 2.35213393E-01	PSI= 5.44413801E-03
X= 6.60000000E-01	R= 6.11608163E-01	Y= 1.20216380E-01	Z= 2.21545588E-01	PSI= 8.47881147E-03
X= 6.60000000E-01	R= 6.16422309E-01	Y= 1.03929839E-01	Z= 2.06028900E-01	PSI= 1.21346707E-02
X= 6.60000000E-01	R= 6.21761643E-01	Y= 8.58665563E-02	Z= 1.88819454E-01	PSI= 1.64440873E-02
X= 6.60000000E-01	R= 6.27603902E-01	Y= 6.61018513E-02	Z= 1.69989012E-01	PSI= 2.14070611E-02
X= 6.60000000E-01	R= 6.33918719E-01	Y= 4.47384543E-02	Z= 1.49635446E-01	PSI= 2.70235921E-02
X= 6.60000000E-01	R= 6.40627903E-01	Y= 2.20408888E-02	Z= 1.28010777E-01	PSI= 3.32936805E-02
X= 6.60000000E-01	R= 6.47147507E-01	Y= -1.53163277E-05	Z= 1.06997152E-01	PSI= 3.97896514E-02
X= 7.20000000E-01	R= 6.49008872E-01	Y= 1.65160838E-01	Z= 2.88087427E-01	PSI= 0.
X= 7.20000000E-01	R= 6.49536208E-01	Y= 1.63495261E-01	Z= 2.86516659E-01	PSI= 3.41887158E-04
X= 7.20000000E-01	R= 6.51050279E-01	Y= 1.58713102E-01	Z= 2.82006711E-01	PSI= 1.36659155E-03
X= 7.20000000E-01	R= 6.53485474E-01	Y= 1.51021600E-01	Z= 2.74753026E-01	PSI= 3.06679722E-03
X= 7.20000000E-01	R= 6.56765790E-01	Y= 1.40660800E-01	Z= 2.64981985E-01	PSI= 5.44413801E-03
X= 7.20000000E-01	R= 6.60775811E-01	Y= 1.27995247E-01	Z= 2.53037383E-01	PSI= 8.47881147E-03
X= 7.20000000E-01	R= 6.65346111E-01	Y= 1.13560067E-01	Z= 2.39423885E-01	PSI= 1.21346707E-02
X= 7.20000000E-01	R= 6.70435765E-01	Y= 9.74845162E-02	Z= 2.24263389E-01	PSI= 1.64440873E-02
X= 7.20000000E-01	R= 6.76028175E-01	Y= 7.98210244E-02	Z= 2.07605342E-01	PSI= 2.14070611E-02
X= 7.20000000E-01	R= 6.82097234E-01	Y= 6.06520513E-02	Z= 1.89527509E-01	PSI= 2.70235921E-02
X= 7.20000000E-01	R= 6.8856804E-01	Y= 4.01233148E-02	Z= 1.70167313E-01	PSI= 3.32936805E-02
X= 7.20000000E-01	R= 6.94939135E-01	Y= 2.00912163E-02	Z= 1.51275485E-01	PSI= 3.97896514E-02
X= 7.20000000E-01	R= 7.01304083E-01	Y= -1.23167902E-05	Z= 1.32316289E-01	PSI= 4.67280386E-02
X= 7.80000000E-01	R= 6.98778666E-01	Y= 1.67874101E-01	Z= 3.14341925E-01	PSI= 0.
X= 7.80000000E-01	R= 6.99271594E-01	Y= 1.66614119E-01	Z= 3.12979142E-01	PSI= 3.41887158E-04
X= 7.80000000E-01	R= 7.00698582E-01	Y= 1.62187590E-01	Z= 3.09033995E-01	PSI= 1.36659155E-03
X= 7.80000000E-01	R= 7.03004416E-01	Y= 1.55358048E-01	Z= 3.02659130E-01	PSI= 3.06679722E-03
X= 7.80000000E-01	R= 7.06123488E-01	Y= 1.46119810E-01	Z= 2.94035929E-01	PSI= 5.44413801E-03
X= 7.80000000E-01	R= 7.09947955E-01	Y= 1.34792296E-01	Z= 2.83462546E-01	PSI= 8.47881147E-03
X= 7.80000000E-01	R= 7.14322554E-01	Y= 1.21835374E-01	Z= 2.71368233E-01	PSI= 1.21346707E-02
X= 7.80000000E-01	R= 7.19210973E-01	Y= 1.07356591E-01	Z= 2.57853377E-01	PSI= 1.64440873E-02
X= 7.80000000E-01	R= 7.24591602E-01	Y= 9.14199524E-02	Z= 2.42977722E-01	PSI= 2.14070611E-02
X= 7.80000000E-01	R= 7.30449774E-01	Y= 7.40689029E-02	Z= 2.26781821E-01	PSI= 2.70235921E-02
X= 7.80000000E-01	R= 7.36751932E-01	Y= 5.54028294E-02	Z= 2.09358444E-01	PSI= 3.32936805E-02
X= 7.80000000E-01	R= 7.42945722E-01	Y= 3.70458796E-02	Z= 1.92223611E-01	PSI= 3.97896514E-02
X= 7.80000000E-01	R= 7.49120716E-01	Y= 1.87682977E-02	Z= 1.75162861E-01	PSI= 4.67280386E-02
X= 7.80000000E-01	R= 7.55460289E-01	Y= -8.59365627E-06	Z= 1.57636044E-01	PSI= 5.42237553E-02
X= 8.40000000E-01	R= 7.48308629E-01	Y= 1.70938064E-01	Z= 3.40868009E-01	PSI= 0.
X= 8.40000000E-01	R= 7.48774593E-01	Y= 1.69638828E-01	Z= 3.39667811E-01	PSI= 3.41887158E-04
X= 8.40000000E-01	R= 7.50132917E-01	Y= 1.65851442E-01	Z= 3.36169130E-01	PSI= 1.36659155E-03
X= 8.40000000E-01	R= 7.52334650E-01	Y= 1.59712399E-01	Z= 3.30498055E-01	PSI= 3.06679722E-03
X= 8.40000000E-01	R= 7.55321601E-01	Y= 1.51383950E-01	Z= 3.22804468E-01	PSI= 5.44413801E-03
X= 8.40000000E-01	R= 7.58997210E-01	Y= 1.41135329E-01	Z= 3.13337079E-01	PSI= 8.47881147E-03
X= 8.40000000E-01	R= 7.63217648E-01	Y= 1.29367575E-01	Z= 3.02466359E-01	PSI= 1.21346707E-02
X= 8.40000000E-01	R= 7.67945558E-01	Y= 1.16184848E-01	Z= 2.90288526E-01	PSI= 1.64440873E-02
X= 8.40000000E-01	R= 7.73159275E-01	Y= 1.01647557E-01	Z= 2.76859384E-01	PSI= 2.14070611E-02
X= 8.40000000E-01	R= 7.78843993E-01	Y= 8.57969824E-02	Z= 2.62217069E-01	PSI= 2.70235921E-02
X= 8.40000000E-01	R= 7.84976411E-01	Y= 6.86980963E-02	Z= 2.46421598E-01	PSI= 3.32936805E-02
X= 8.40000000E-01	R= 7.91041936E-01	Y= 5.17857271E-02	Z= 2.30798427E-01	PSI= 3.97896514E-02
X= 8.40000000E-01	R= 7.97127448E-01	Y= 3.48176263E-02	Z= 2.15123772E-01	PSI= 4.67280386E-02
X= 8.40000000E-01	R= 8.03274085E-01	Y= 1.76790947E-02	Z= 1.99291677E-01	PSI= 5.42237553E-02
X= 8.40000000E-01	R= 8.09616659E-01	Y= -5.76366770E-06	Z= 1.82954902E-01	PSI= 6.22768016E-02

END THIS CASE, HALLELUJAH

Complete Program

```
PROGRAM D1290.(INPUT=1001,OUTPUT=1001,TAPE5=INPUT,TAPE6=OUTPUT,  
1 TAPE8,TAPE9,TAPE10,TAPE11,TAPE12,TAPE13)
```

B SHOCK GEOMETRY

SHOCK

BODY

Z

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APPENDIX A - Continued

```

C   PINF = FREE STREAM PRESSURE, DYNES/ CM**2
C   TINF = FREE STREAM TEMPERATURE, DEG.K
C   VINP = FREE STREAM VELOCITY, CM/SEC
C   MUI  = MOLECULAR WEIGHT FOR EACH SPECIES, GM/MOLE
C   THETA I = CHARACTERISTIC VIBRATIONAL TEMPERATURE, DEG.K
C   DGENI = FUDGE FACTOR TO PERMIT APPROXIMATING POLYATOMIC MOLECULE
C         BY DIATOMIC MOLECULE
C   FI   = 0 FOR MONATOMIC SPECIES
C         = 1 FOR ALL OTHERS
C   DELHI = HEAT OF FORMATION, ERGS/MOLE
C   DELI  = DISSOCIATION ENERGY OF SPECIES
C   EVI   = VIBRATIONAL ENERGY OF SPECIES
C   LI    = NUMBER OF ELECTRONIC LEVELS FOR EACH SPECIES LI.LE.20
C   GIL   = DEGENERACY OF L-TH ELECTRONIC LEVEL FOR I-TH SPECIES
C   EPSIIL = L-TH ELECTRONIC ENERGY LEVEL FOR I-TH SPECIES
C   AJ    = FREQUENCY FACTOR IN ARRHENIUS TYPE RATE EQ.
C   BJ    = TEMPERATURE EXPONENT IN ARRHENIUS TYPE RATE EQ.
C   EJ    = IN ARRHENIUS TYPE RATE EQ.
C   AIJ   = FACTOR TO ALLOW USE OF GENERAL SPECIES IN REACTION EQS IF
C           DESIRED, =1.0 OR =0.0
C   NUIJ  = STOICHIOMETRIC COEFFICIENTS OF I-TH REACTANT IN J-TH
C           REACTION
C   NUPIJ = STOICHIOMETRIC COEFFICIENT FOR I-TH PRODUCT IN J-TH
C           REACTION
C   ALPIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
C   BETAIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
C   SIGIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
C   XI    = INITIAL COMPUTING INTERVAL, .0001220703125 UNLESS INPUT
C   ELE1  = (2*IMAX+1) VALUES USED BY INTEGRATION SCHEME
C           NORMALLY .1,.5 OR .05
C   ELE2  = (2*IMAX+1) VALUES USED BY INTEGRATION SCHEME
C           NORMALLY .05,.1 OR .01 AND .LT.ELE1
C   XPST  = 99 OR LESS X-S AT WHICH PHYSICAL SPACE CALCULATIONS ARE
C           DESIRED. THEY MUST BE MULTIPLES OF DELX IN ORDER TO
C           HAVE RS,COST,ZS AND SINT VALUES
C           AND LAST MUST BE .GT.X AT ZTERM
C           THEREFORE, XPST(NXPST) SET = X AT ZTERM + 100.0 IN
C           PROGRAM
C           XPST(1) MAY NOT BE 0.0
C           THEREFORE, XPST(1) SET = DELX IN PROGRAM
C   NXPST = NUMBER OF X-S AT WHICH PHYSICAL SPACE CALCULATIONS ARE
C           DESIRED
C   IPF   = PRINT FREQUENCY, 3 UNLESS INPUT OTHERWISE
C           IPF NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP RUN
C   CIMAX = MAXIMUM CJ OR COMPUTING INTERVAL
C           0.0625 UNLESS INPUT OTHERWISE
C           CIMAX NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP
C           RUNS
C   TIMER = TIME, IN DECIMAL SECONDS, REQUESTED ON JOB CARD
C           IF THE JOB DOES NOT TERMINATE IN THE TIME ESTIMATED ON
C           THE JOB CARD, DATA FOR PICKUP WILL BE STORED ON TAPE 13.
C           IT IS = 3600.0 OR 1 HOUR UNLESS INPUT OTHERWISE
C           TIMER NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP
C           RUNS
C   IPICKUP = 0 UNLESS INPUT
C           = 1 TO PICKUP CASE FROM TAPE 13
C   HCHECKT = CONTROL ON SIZE OF COMPUTING INTERVAL IN CHECK
C           IF(ABS(HPREV-H)/H.GT.HCHECK) REDUCE INTERVAL
C   TCHECKT = CONTROL ON SIZE OF COMPUTING INTERVAL IN CHECK
C           IF(ABS(TPREV-T)/T.GE.TCHECK) REDUCE INTERVAL
C   PHMAX  = CONTROL ON COMPUTING INTERVAL .LE.65.0
C   $
C
C   AFTER READING IN NAM1, READ IN THE IMAX SPECIES BY FORMAT(8A10)
C   10 SPACES PER SPECIES
C   THEN READ IN THE JMAX REACTIONS BY THE SAME FORMAT USING 20

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APPENDIX A - Continued

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C      SPACES PER REACTION
C      IF THE SPECIES AND REACTIONS ARE NOT READ IN,
C      IMAX/8 PLUS JMAX/4 BLANK CARDS MUST BE PUT IN THE DECK
C
C      STOPS
C      STOP 1 INCORRECT INPUT
C      STOP 6 EOF 10 IN MAIN
C      STOP 13 IN SHOCKG
C      STOP 30 IN CHECK WHEN COMPUTING INTERVAL.LT.1.0E-15
C      STOP 50 EOF 9 IN FDPDX
C      STOP 66 IN BASIC WHEN NO CONVERGENCE ON E ITERATION
C      STOP 301 IN MAIN FOR ERROR IN XPST ARRAY OR IZTERM.GT.500
C      STOP 321 ITR1 STOP IN MAIN
C      STOP 422 IN MAIN AFTER PICKUP TAPE WRITTEN
C      STOP 563 IN MAIN WHEN X.NE.VARI(IPSII)
C      STOP 665 IN MAIN AFTER AN INTEGRATION ATTEMPT
C      STOP 670 IN MAIN WHEN A CI NEGATIVE
C
C      COMMON M,IX,IMAX,IPSI,IBUG(15)
C      COMMON P( 500),DPOX( 500),VARI( 500)
C      FOLLOWING 7 VARIABLES DIMENSIONED BY IMAX
C      COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
1      LI(25)
C      COMMON R,MUINF,DELTA,LAMSQ,OMEGSQ,OMEGA,MU,T,U
C      FOLLOWING 2 VARIABLES DIMENSIONED BY (LMAX IN LI,IMAX)
C      COMMON EPSIIL(20,25),GIL(20,25)
C      COMMON VAR(52),CUVAR(52),DER(51)
C
C      COMMON ZS,RS,RC,SINT,COST,PS,US,PSIS
C      FOLLOWING 4 VARIABLES DIMENSIONED BY JMAX
C      COMMON MJ(50),EJ(50),AJ(50),BJ(50)
C      FOLLOWING 3 VARIABLES DIMENSIONED BY IMAX
C      COMMON TVI(25),NI(25),DGENI(25)
C      FOLLOWING 3 VARIABLES DIMENSIONED BY (IMAX+1,JMAX) OR
C      (IMAX ,JMAX)
C      COMMON NUIJ(26,50),AIJ(25,50),NUIPJ(25,50)
C      FOLLOWING 3 VARIABLES DIMENSIONED BY (IMAX,IMAX)
C      COMMON SIGIK(25,25),ALPIK(25,25),BETAIK(25,25)
C      COMMON KSTAG,IMAXP2,IMAXL,N,IG,ISTAG,LPS2,LPS1,IMAXP1
C      COMMON X,TS,ES,RHOS,HS,RHOVRT,PHMAX,AAAAA,PREPSIS,PREX,PRERU
C      EVIS(IMAX)
C      COMMON EVIS(25),XPST(100)
C
C      COMMON /LAB2/ DELX,ZSTERM,IZTERM
C      COMMON /LAB3/ EINF,PINF,RHOINF,VINF,E,JMAX,KEYINT,RHO,HSTAG
C      COMMON /LAB4/ PFTL,KITR1,EITR1
C      COMMON /LAB5/ IUNEG
C      COMMON /LAB6/ ELB,SPEC,CJ,TPREV,HPREV,HCHECK,TCHECK
C      COMMON /LAB7/ ITNEG,IEXP
C      COMMON /LAB8/ ELE1(51),ELE2(51),NERR
C      SPECIE(IMAX),REACT(JMAX),DELI(IMAX)
C      DIMENSION SPECIE(25),REACT(50),IN(8),DELI(25)
C
C      DOUBLE PRECISION VAR,XVAR,H,CI,EVI
C
C      DIMENSION RUT(200),PSISTG(200)
C      DIMENSION ENG(11),ENGI(11)
C      DIMENSION CIG(25,6),EIG(25,6)
C      DIMENSION PSIG(6),TG(6),HG(6),CIT(6),EIT(6),EG(6)
C      CM(IMAX),CI(IMAX),EVI(IMAX)
C      DIMENSION CM(25 ),CI(25 ),EVI(25 )
C      DIMENSION XX(3),XXX(3)
C      XX AND XXX ARE TOKEN DIMENSIONS WHICH WILL CHANGE AS THE
C      DIMENSION STATEMENTS ARE CHANGED...THEY ARE USED FOR PICKUP RUN
C

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APPENDIX A - Continued

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EQUIVALENCE (VAR(1),XVAR),(VAR(2),H),(VAR(3),CI(1))
C      VAR(2+IMAX+1)=EVI(1)
EQUIVALENCE(M,XX(1)),(DELX,XXX(1))
C
REAL MUI,LAMSO,MUINF,MU
REAL NI
REAL MINF,MINFSQ,LAMBDA
REAL NUIJ,NUPIJ
C
C      INPUT
C
NAME LIST/NAM1/ DELX,ZTERM,IMAX,JMAX,IBUG,MJ,M,R,GAMMA,
1 CIINF,PINF,TINF,VINF,MUI,THETA1,DGENI,FI,DELHI,DELI,EVI,LI,
2 GIL,EPSIIL,AJ,BJ,EJ,AIJ,NUIJ,NUPIJ,ALPIK,BETA1K,SIGIK,XI,CIMAX,
3 ELE1,ELE2,XPST,NXPST,IPF,TIMER,IPICKUP,HCHECKT,TCHECKT,PHMAX
C
EXTERNAL FOFTS
C      INITIALIZE
REWIND 8
REWIND 9
REWIND 10
REWIND 11
REWIND 12
-----
REWIND 13
NERR=0
C
C      TIMER= ONE HOUR
TIMER=3600.0
DO 5 I=1,15
5  IBUG(I)=1
NXPST=2
IPICKUP=0
ICHEK=0
ITNEG=0
IEXP=0
NEG=0
IGK=0
IUNEG=0
DELZS=.001952125
DELX=.015625
XI=.0001220703125
CIMAX=.0625
IPF=5
DO 10 I=1,52
VAR(I)=0.
CUVAR(I)=0.
IF (I.EQ.52) GO TO 10
DER(I)=0.
ELE1(I)=0.
ELE2(I)=0.
10 CONTINUE
C      READ INPUT
C      READ (5,15) (IN(I),I=1,8)
15  FORMAT (8A10)
READ (5,NAM1)
IF (IPICKUP.EQ.0) GO TO 60
PRINT 15, (IN(I),I=1,8)
READ PICKUP FROM TAPE13
C      THIS SHOULD PICKUP ALL COMMON AND LABELED COMMON
C      PLEASE CHECK DIMENSIONS IF THERE ARE PICKUP PROBLEMS
C
READ (13) (XX(I),I=1,8961),(XXX(I),I=1,128)
DO 20 I=1,IZTERM
READ (13) X,ZS,RS,RC,COST,SINT
CALL REOUT (10,1,0,X,ZS,RS,RC,COST,SINT)
READ (13) (DPDX(J),J=I,IZTERM)

```

APPENDIX A - Continued

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CALL RECOUT (8,2,0,DPDX,I,IZTERM,1)
READ (13) IX,TS,ES,PS,RHOS,US,PSIS,HS
READ (13) (EVIS(J),J=1,IMAX)
CALL RECOUT (11,1,0,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECOUT (11,2,0,EVIS,1,IMAX,1)
READ (13) X
READ (13) (P(J),J=1,IZTERM)
CALL RECOUT (9,1,0,X)
CALL RECOUT (9,2,0,P,1,IZTERM,1)
20 CONTINUE
IF (KSTAG.EQ.0) GO TO 30
DO 25 I=1,KSTAG
READ (13) K,RHOURT,VAR(1),PSIS
CALL RECOUT (12,1,0,K,RHOURT,VAR(1),PSIS)
25 CONTINUE
30 REWIND 8
REWIND 9
REWIND 10
REWIND 11
REWIND 13
IREAD=IPSI
IF (IPSI.EQ.6.AND.ISTAG.EQ.1) IREAD=IPSI-1
DO 35 I=1,IREAD
CALL RECIN (11,1,IRECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
35 CONTINUE
DO 40 I=1,IREAD
CALL RECIN (9,1,IRECIN,X)
CALL RECIN (9,2,IRECIN,P,1,IZTERM,1)
CALL RECIN (8,2,IRECIN,DPDX,I,IZTERM,1)
40 CONTINUE
READ (13) (XX(I),I=1,8961),(XXX(I),I=1,128)
REWIND 13
PRINT 45
45 FORMAT (24H1----- PICKUP CASE -----/)
PRINT 50, IMAXL,(XPST(I),I=1,10),(ELE2(I),I=1,5)
50 FORMAT (1X,6HIMAXL=,I3/,1X,5HXPST=,2(5E17.8/)/1X,5HELE2=,5E17.8/1X
1,6HKSTAG=,I3/)
PRINT 600, IPSI,IX,XVAR,H,MU,PFTL,RHO,U,T,E,SPEC,SUMCI
IMAXP1=IMAX+1
PRINT 605, (VAR(I),I=3,IMAXP1)
PRINT 610, (CM(I),I=1,IMAX)
IMAXP3=2+IMAX+1
PRINT 615, (VAR(I),I=IMAXP3,IMAXL)
SPEC=0
IX=IX-1
IBUG(11)=0
KEYINT=0
KIPF=IPF-1
HCHECK=HCHECKT
TCHECK=TCHECKT
PRINT 55, IPF,CIMAX,TIMER,HCHECKT,TCHECKT,IZTERM,KSTAG
55 FORMAT (10H IPF=I2,10H CIMAX=E15.8,10H TIMER=E15.8,10H
1 HCHECKT=E15.8,10H TCHECKT=E15.8/10H IZTERM=I2,10H KSTAG=I3/
2)
GO TO 560
60 CONTINUE
C
IF (IBUG(1).EQ.1) GO TO 65
WRITE (6,NAM1)
65 PRINT 70
70 FORMAT (1H1)
PRINT 15, (IN(I),I=1,8)
C
C SUM OF CIINF SHOULD BE 1.0
SUM=0.

```

APPENDIX A - Continued

```

DO 75 I=1,IMAX
75  SUM=SUM+CIINF(I)
    IF (SUM.EQ.1.0) GO TO 85
    PRINT 80, SUM,(CIINF(I),I=1,IMAX)
80  FORMAT (34H SUM OF CIINF SHOULD BE 1.0. IT IS,E17.8,8H CIINF=/5(5
    E17.8))
    STOP 1
C
85  CONTINUE
    HCHECK=HCHECKT
    TCHECK=TCHECKT
C    READ IN SPECIES AND REACTIONS
    READ (5,90) (SPECIE(I),I=1,IMAX)
90  FORMAT (8A10)
    PRINT 95
95  FORMAT (//)
    PRINT 100
100  FORMAT (12H SPECIES/)
    DO 110 I=1,IMAX
105  FORMAT (15,A10)
110  PRINT 105, I,SPECIE(I)
    PRINT 95
    JMAX2=2*JMAX
    READ (5,90) (REACT(I),I=1,JMAX2)
    PRINT 115
115  FORMAT (14H REACTIONS/)
    J=0
    DO 120 I=1,JMAX2,2
    J=J+1
120  PRINT 125, J,REACT(I),REACT(I+1)
125  FORMAT (15,2A10)
    PRINT 95
C    PRINT INPUT
    PRINT 130, IPF
130  FORMAT (17H PRINT FREQUENCY=I3)
    PRINT 135, HCHECKT,TCHECKT,PHMAX
135  FORMAT (10H HCHECKT=E15.8,10H TCHECKT=E15.8,10H PHMAX=E15.8)
    NXPSTP1=NXPST+1
    PRINT 140, XI,CIMAX,ELE1,ELE2,NXPST,(XPST(I),I=1,NXPSTP1)
140  FORMAT (4H XI=E15.8/7H CIMAX=E15.8/6H ELE1=2E17.8/7(7E17.8/)/6H EL
    E2=2E17.8/7(7E17.8/)/7H NXPST=I3/6H XPST=/15(7E17.8/)/)
    PRINT 145, DELX,ZSTERM,TIMER,IPICKUP
145  FORMAT (6H DELX=E15.8/8H ZSTERM=E15.8/7H TIMER=E15.8/9H IPICKUP=I1
    1//)
    PRINT 150, IMAX,JMAX,M,R,GAMMA,PINF,TINF,VINF,IBUG
150  FORMAT (6H IMAX=I2,8H JMAX=I2,5H M=I1/3H R=E15.8/7H GAMMA=E15.
    18/6H PINF=E15.8/6H TINF=E15.8/6H VINF=E15.8/6H IBUG=I1,14I5/)
    PRINT 155
155  FORMAT (5X,3HMUI12X,6HTHETA19X,5HDGENI10X,2HF113X,5HDELHI10X,4HDEL
    1I11X,5HCIINF10X,3HEVI12X,2HLI/)
    DO 165 I=1,IMAX
160  FORMAT (7E15.5,0I5.6,I5)
165  PRINT 160, MUI(I),THETA1(I),DGENI(I),FI(I),DELHI(I),DELI(I),CIINF(
    I),EVI(I),LI(I)
    PRINT 170
170  FORMAT (/6X,2HMJ6X,2HAJ16X,2HBJ16X,2HEJ/)
    DO 180 J=1,JMAX
175  FORMAT (18,3E18.8)
180  PRINT 175, MJ(J),AJ(J),BJ(J),EJ(J)
    PRINT 95
    IMAXP1=IMAX+1
    DO 225 I=1,IMAX
    PRINT 185, I,(GIL(L,I),L=1,IMAXP1)
185  FORMAT (4H I=I5,23H (GIL(L,I),L=1,IMAX+1)/(3(7E18.8/)))

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APPENDIX A - Continued

```

PRINT 190, I, (EPSIIL(L, I), L=1, IMAXP1)
190  FORMAT (4H I=I5, 26H (EPSIIL(L, I), L=1, IMAX+1)/3(7E18.8/))
PRINT 195, I, (AIJ(I, J), J=1, JMAX)
195  FORMAT (4H I=I5, 21H (AIJ(I, J), J=1, JMAX)/5(7E18.8/))
PRINT 200, I, (ALPIK(K, I), K=1, IMAX)
200  FORMAT (4H I=I5, 23H (ALPIK(K, I), K=1, IMAX)/3(7E18.8/))
PRINT 205, I, (BETAIK(K, I), K=1, IMAX)
205  FORMAT (4H I=I5, 24H (BETAIK(K, I), K=1, IMAX)/3(7E18.8/))
PRINT 210, I, (SIGIK(K, I), K=1, IMAX)
210  FORMAT (4H I=I5, 23H (SIGIK(K, I), K=1, IMAX)/3(7E18.8/))
PRINT 215, I, (NUIJ(I, J), J=1, JMAX)
215  FORMAT (4H I=I5, 22H (NUIJ(J, I), J=1, JMAX)/5(7E18.8/))
PRINT 220, I, (NUPIJ(I, J), J=1, JMAX)
220  FORMAT (4H I=I5, 23H (NUPIJ(J, I), J=1, JMAX)/5(7E18.8/))
PRINT 95
225  CONTINUE
IM=IMAX+1
PRINT 215, IM, (NUIJ(IM, J), J=1, JMAX)
PRINT 230
230  FORMAT (2X, 9HEND INPUT//)
PRINT 95

C
C      DEFINE SHOCK GEOMETRY
C      AT EACH X FIND ZS, RS, RC, COST, SINT AND STORE ON TAPE 10
C
CALL SHOCKG (DELX, ZSTERM, IZTERM)

C
C      IZTERM=NUMBER OF DELTA X INCREMENTS AS GENERATED IN SHOCKG
IF (NXPST-1.GT.IZTERM) PRINT 235
235  FORMAT (84H NXPST-1.GT.IZTERM, IT MUST BE .LE. FOR PHYSICAL SPACE C
1ALCULATIONS - SEE DO 700 LOOP/)
IF (NXPST-1.GT.IZTERM) STOP 301
PRINT 415, IZTERM
IF (IZTERM.GT.500) PRINT 240
240  FORMAT (1X, 50HIZTERM.GT.500 CHANGE DIMENSION OF P, OPDX AND VARI )
IF (IZTERM.GT.500) STOP 301

C
C
C      STOP 301
C      FREESTREAM QUANTITIES
SUM=0
DO 245 I=1, IMAX
245  SUM=SUM+CIINF(I)/MUI(I)
MUINF=1./SUM
RHOINF=MUINF*PINF/(R*TINF)
AINF=SQRT(GAMMA*R*TINF/MUINF)
MINF=VINF/AINF
C      FOR EACH I, SPECIE
EINF=0
DO 275 I=1, IMAX
TEM=EXP(THETAI(I)/TINF)
EVIINF(I)=(R*THETAI(I))/(MUI(I)*(TEM-1.))*FI(I)
C      FOR EACH L, REACTION LEVEL
GSUM=0
GESUM=0
LII=LI(I)
IF (LII.LE.20) GO TO 255
PRINT 250, LII
250  FORMAT (1X, 4HLII=, I3, 2X, 28HA LEVEL IN LI ARRAY IS GT 20/2X, 43HNEED
1 TO CHANGE DIMENSION OF EPSIIL AND GIL )
255  CONTINUE
DO 265 L=1, LII
TEM1=EXP(-EPSIIL(L, I)/TINF)
GSUM=GSUM+GIL(L, I)*TEM1
GESUM=GESUM+GIL(L, I)*EPSIIL(L, I)*TEM1
IF (IBUG(1).NE.0) GO TO 265
PRINT 260, I, L, GSUM, GESUM, TEM1, EPSIIL(L, I), TINF, GIL(L, I)
260  FORMAT (36H I, L, GSUM, GESUM, TEM1, EPSIIL, TINF, GIL/215.6E18.8/)

```

APPENDIX A - Continued

```

265  CONTINUE
      EEIINF=R/MUI(I)*(GESUM/GSUM)
      EIINF=1.5*R*TINF/MUI(I)+FI(I)*R*TINF/MUI(I)+EVIINF(I)+EEIINF+DELHI
      1(I)/MUI(I)
      EINF=EINF+EIINF*CIINF(I)
      IF (IBUG(2).NE.0) GO TO 275
      PRINT 270, I,EINF,TEM,THETA1(I),TINF,MUI(I),EVIINF(I),GSUM,GESUM,E
      1EIINF,EIINF,FI(I),DELHI(I)
270  FORMAT (34H I,EINF,TEM,THETA1,TINF,MUI,EVIINF/15.6E18.8/33H GSUM,G
      1ESUM,EEIINF,EIINF,FI,DELHI/6E18.8/)
275  CONTINUE
      PRINT 280, MUINF,RHOINF,AINF,MINF,EIINF,EINF,EEIINF
280  FORMAT (31H +++ FREESTREAM QUANTITIES +++/8H MUINF=E15.8,10H R
      1HOINF=E15.8,8H AINF=E15.8,8H MINF=E15.8,9H EIINF=E15.8/7H E
      2INF=E15.8/9H EEIINF=/(8E18.8/))
      PRINT 285, (EVIINF(I),I=1,IMAX)
285  FORMAT (9H EVIINF=/(6E18.8))
C
C                                     END FREESTREAM QUANTITIES
C                                     BEGIN QUANTITIES BEHIND SHOCK
C                                     FOR RANGE OF X
C
      PRINT 290
290  FORMAT (/33H +++ QUANTITIES BEHIND SHOCK +++/6X,2HTS15X,2HES16X,
      12HPS16X,4HRHOS14X,2HUS16X,4HPSIS14X,2HHS)
      IEOF=10
      IF (NXPST.EQ.2) PRINT 310
      IF (NXPST.EQ.2) STOP 2
      NXPSTM1=NXPST-1
      ITK=0
      DO 305 IX=1,IZTERM
C
C      USE RECOUT TO WRITE
C      USE RECIN TO READ
C
      CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
      IF (ENDFILE 10) 295,305
295  PRINT 300, IEOF
300  FORMAT (14H IN MAIN EOF 13)
      STOP 6
C
C                                     STOP 6
305  CONTINUE
310  FORMAT (78H NXPST=2 - SURELY SOME PHYSICAL SPACE VALUES ARE DESIRE
      1D -- MAKE IT 3 AT LEAST)
      DO 315 IT=2,NXPSTM1
      IF (ABS(XPST(IT)-X).GT.0.000001) GO TO 315
      ITK=ITK+1
315  CONTINUE
      TEM=SINT**2
      LAMBDA=RHOINF*VIN*F*SINT
      OMEGA=PINF+RHOINF*VIN*F**2*TEM
      DELTA=EINF+PINF/RHOINF+(VIN*F**2*TEM)/2.
      LAMSQ=LAMBDA**2
      OMEGSQ=OMEGA**2
      MINFSQ=MINF**2
      TEM=TEM*MINFSQ
      TG=(TINF*(2.*GAMMA*TEM-(GAMMA-1.0))*((GAMMA-1.0)*TE4+2.))/((GAMMA+
      11.)***2*TEM)
      IF (IBUG(5).NE.0) GO TO 325
      PRINT 320, X,SINT,LAMBOA,OMEGA,DELTA,TEM,TG
320  FORMAT (39H X, SINT, LAMBDA, OMEGA, DELTA, TEM, TG/7E17.8/)
C
C                                     C5.002 LF-ITR1
325  CONTINUE
      DELTTS=10.

```

APPENDIX A - Continued

```

E1=.0001
E2=.001
MAXI=50
CALL ITR1 (TG,DELTT,FOFTS,E1,E2,MAXI,ICODE)
IF (ICODE.EQ.1) PRINT 330
330  FORMAT (34H MAXIMUM ITERATION EXCEEDED *****/)
IF (ICODE.EQ.2) PRINT 335
335  FORMAT (30H DERIVATIVE =0. IN ITR1 *****/)
IF (ICODE.EQ.1.OR.ICODE.EQ.2) STOP 321
C
TS=TG
ES=0.
DO 360 I=1,IMAX
IF (M.EQ.1) EVIS(I)=EVIINF(I)
IF (M.EQ.1) GO TO 345
TEM=EXP(THETA(I)/TS)
EVIS(I)=(R*THETA(I))/(MUI(I)*(TEM-1.))*FI(I)
IF (IBUG(5).NE.0) GO TO 345
PRINT 340, IX,I,TEM,EVIS(I)
340  FORMAT (19H IX,I,TEM,EVIS(I)=2I5,2E18.8)
345  SUMG=0.
SUMGE=0.
LII=LI(I)
DO 350 L=1,LII
TEM1=EXP(-EPSIIL(L,I)/TS)
SUMG=SUMG+TEM1*GIL(L,I)
350  SUMGE=SUMGE+TEM1*GIL(L,I)*EPSIIL(L,I)
EEIS=(R/MUI(I))*(SUMGE/SUMG)
EIS=(1.5*R*TS)/MUI(I)+(FI(I)*R*TS)/MUI(I)+1.0*EVIS(I)+EEIS+DELHI(I)
IF (IBUG(5).NE.0) GO TO 360
PRINT 355, EEIS,EIS,SUMG,SUMGE
355  FORMAT (22H EEIS,EIS,SUMG,SUMGE=4E18.8)
360  ES=ES+EIS*CIINF(I)
PS=SQRT(OMEGSQ-2.*LAMSQ*(DELTA-ES))
RHOS=(MUIINF*PS)/(R*TS)
US=VINFCOST
PSIS=(RHOINF*VINFRS**2)/2.
HS=PS/RHOS+ES
C
C      WRITE ON TAPE 11 AT EACH X
CALL REOUT (11,1,0,IX,YS,ES,PS,RHOS,US,PSIS,HS)
CALL REOUT (11,2,0,EVIS,1,IMAX,1)
C
PRINT 365, TS,ES,PS,RHOS,US,PSIS,HS
365  FORMAT (/7E18.8)
PRINT 370, IX,(EVIS(I),I=1,IMAX)
370  FORMAT (5H IX=I3,7H EVIS=/4(7E18.8)/)
IF (IBUG(5).NE.0) GO TO 385
PRINT 375
375  FORMAT (50H //////////////////////////////////////)
PRINT 380, IX,TS,PS,RHOS,US,PSIS,HS,ES
380  FORMAT (29H IX,TS,PS,RHOS,US,PSIS,HS,ES/I4,7E18.8/)
385  CONTINUE
REWIND 10
END FILE 11
REWIND 11
PRINT 390, ITK,NXPST
390  FORMAT (/2X,10HXXXXX ITK=I3,2X,6HNXPST=I3,2X,5HXXXXX/)
IF (ITK.GE.3*NXPST/4) GO TO 400
PRINT 395
395  FORMAT (89H NUMBER OF X-S IN XPST ARRAY,ITK,IS .LT. 3*NXPST/4 - R
1EEXAMINE DELX,NXPST AND XPST ARRAY)
C
C      SECOND STOP 301
STOP 301
400  CONTINUE

```

APPENDIX A - Continued

```

C          END COMPUTATION OF QUANTITIES BEHIND SHOCK
C
C      CALL FPODX
C          FIND PRESSURE,P, AT EACH X FOR EACH STREAMLINE AND
C          STORE ON TAPE 9
C          FIND P.DOT, DPOX, AT EACH X FOR EACH STREAMLINE AND
C          STORE ON TAPE 8
C
C          INTEGRATE ALONG EACH STREAMLINE PSI
C
C          VAR(1) = XVAR
C          VAR(2)= H, ENTHALPY          VAR(2) MUST BE H, WHICH MAY BE + OR -
C                                     CONCENTRATION OF SPECIE
C          VAR(3) = CI(1)
C          -
C          VAR(2+IMAX)=CI(IMAX)
C                                     EQUILIBRIUM VIBRATIONAL ENERGY
C          VAR(2+IMAX+1)=EVI(1)
C          -
C          VAR(2+IMAX+IMAX)=EVI(IMAX)
C
C      DO 410 I=1,IMAX
C          TRUNCATE
C          Y=FI(I)*(DELI(I)/THETA(I)+1.0)
C          NI(I)=AINT(Y)
C
C          IF (IBUG(5).NE.0) GO TO 410
C          PRINT 405, I,Y,NI(I)
405      FORMAT (12H I,Y,NI(I)=I5,2E18.8/)
410      CONTINUE
C
C          MU=0.
C          N=1+2*IMAX
C          IF (M.EQ.0) N=N-IMAX
C
C          INITIALIZE
C          PRINT 415, IZTERM
415      FORMAT (9H IZTERM=I3)
C          KSTAG=0
C          ISTAG=0
C          XPST(1)=DELX
C          XPST(NXPST)=VARI(IZTERM)+100.0
C          SUMCI=0.
C          PRINT 95
C          IZTM1=IZTERM-1
C          LPSI=1
C
C          IPSI=0
C          BEGIN EACH STREAMLINE COMPUTATION HERE
420      IPSI=IPSI+1
C          IF (IPSI.EQ.IZTERM) GO TO 735
425      CONTINUE
C          KIPF=0
C          IEOF=11
C          ISTAG = 2 FOR STREAMLINE DELX
C          IF (ISTAG.EQ.1) ISTAG=2
C          CALL RECIN (11,1,IRECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
C          CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
C          IF (ENDFILE 11) 430,440
430      PRINT 435, IEOF,IPSI
435      FORMAT (5H EOFI4,57H IN MAIN, TRY TO COMPUTE PHYSICAL SPACE VALU
C          IES --- IPSI=I3//)
C          GO TO 735
440      CONTINUE

```

APPENDIX A - Continued

```

C      IF (IPSI.EQ.1) HSTAG=HS
C
C      CJ=XI
C      SPEC=0.0
C      EVALUATE DERIVATIVES WHEN SPEC=0.0
C      II=0
C      USE SHOCK VALUES FOR INITIAL COMPUTATION ON EACH STREAMLINE
C      KEYINT=0
C      IX=0
C      T=TS
C      IF (M.EQ.0) GO TO 450
C      DO 445 I=1,IMAX
445    TVI(I)=TINF
C      GO TO 450
450    DO 455 I=1,IMAX
455    TVI(I)=TS
460    RHO=RHOS
C      MU=MUINF
C      U=US
C      DO 465 I=1,IMAX
C      MM=2+I
C      K=IMAX+MM
C      VAR(MM)=0.
C      VAR(MM)=CIINF(I)
C      VAR(K)=0.
C      IF (M.EQ.0) VAR(K)=EVIS(I)
C      IF (M.EQ.1) VAR(K)=EVIINF(I)
C      EVI(I)=VAR(K)
465    CONTINUE
C      E=ES
C      H=HS
C      IF (IPSI.EQ.6.AND.ISTAG.EQ.0) GO TO 635
C
C      IEOF=9
C      CALL RECIN (9,1,IRECIN,X)
C      CALL RECIN (9,2,IRECIN,P,IPSI,IZTERM,1)
C      IF (ENDFILE 9) 430,470
C
C      IEOF=8
470    CALL RECIN (8,2,IRECIN,DPOX,IPSI,IZTERM,1)
C      IF (ENDFILE 8) 430,475
475    IF (IBUG(3).NE.0) GO TO 485
C      PRINT 480, (VARI(IT),DPOX(IT),P(IT),IT=IPSI,IZTERM)
480    FORMAT (33H (DPOX(IT),P(IT),IT=IPSI,IZTERM)/(6E17.8))
485    CONTINUE
C      VAR(1)=X
C      OMIT PSI=0.0 STREAMLINE FOR NOW --- PICK IT UP LATER
C      IF (X.NE.0.) GO TO 490
C      IG=0
C      PRINT 725
C      GO TO 730
C
C      CONTINUE
490    IF (X.EQ.VARI(IPSI)) GO TO 500
C
C      PRINT 495, IPSI,X,VARI(IPSI)
495    FORMAT (6H IPSI=I4.4H X=E15.8,13H VARI(IPSI)=E15.8,34H X AND VA
1RI(IPSI) SHOULD BE EQUAL/63H EXAMINE GENERATION OF X,ON TAPE 9,AN
2DVARI IN FPODX SUBROUTINE)
C      STOP 663
C
C
C      CONTINUE
C      INITIALIZE
C

```

STOP 663

APPENDIX A - Continued

```

ELB=0
SPEC=0
IF (VAR(1).GT.XPST(LPS1)) LPS1=LPS1+1
LPS2=LPS1
505 CONTINUE
C
C CHECK ON PICKUP
CALL SECOND (CHECKT)
IF (IX.NE.1) GO TO 515
PRINT 510, CHECKT
510 FORMAT (20H -----CHECKT=E15.8)
515 IF (ICHECK.EQ.1) GO TO 540
IF ((TIMER-CHECKT).GT.30.) GO TO 560
IF (IPSI.GT.5) GO TO 525
PRINT 520
520 FORMAT (1X,/10X,10H$$$$$$$$$/67H MUST BE ON OR BEYOND PSI=0.,
1 IPSI=6, BEFORE PICKUP IS POSSIBLE/10X,10H$$$$$$$$$/)
525 CONTINUE
KIPF=0
IPF=1
C
WRITE PICKUP TAPE
WRITE (13) (XX(I),I=1,8961),(XXX(I),I=1,128)
PRINT 530, TIMER,CHECKT
530 FORMAT (30H PICKUP TAPE WRITTEN -- TIMER=E15.8,10H CHECKT=E15.8/
1)
ICHECK=1
PRINT 600, IPSI,IX,XVAR,H,MU,PFTL,RHO,U,T,E,SPEC,SUMCI
PRINT 605, (VAR(I),I=3,IMAXP2)
PRINT 610, (CM(I),I=1,IMAX)
IMAXP3=2+IMAX+1
PRINT 615, (VAR(I),I=IMAXP3,IMAXL)
PRINT 620
PRINT 535
535 FORMAT (/93H -----
1 -----//)
ITEST=0
540 IF (TIMER-CHECKT.GT.10.) GO TO 560
REWIND 8
REWIND 9
REWIND 10
REWIND 11
REWIND 12
DO 545 I=1,IZTERM
C READ
C WRITE ON 13 TO SAVE FOR PICKUP
CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
WRITE (13) X,ZS,RS,RC,COST,SINT
CALL RECIN (8,2,IRECIN,DPOX,I,IZTERM,1)
WRITE (13) (DPOX(J),J=1,IZTERM)
CALL RECIN (11,1,IRECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
WRITE (13) IX,TS,ES,PS,RHOS,US,PSIS,HS
WRITE (13) (EVIS(J),J=1,IMAX)
CALL RECIN (9,1,IRECIN,X)
CALL RECIN (9,2,IRECIN,P,I,IZTERM,1)
WRITE (13) X
WRITE (13) (P(J),J=1,IZTERM)
545 CONTINUE
DO 550 I=1,KSTAG
CALL RECIN (12,1,IRECIN,IPSI,RHOURT,VAR(1),PSIS)
WRITE (13) IPSI,RHOURT,VAR(1),PSIS
550 CONTINUE
PRINT 50, IMAXL,(XPST(I),I=1,10),(ELE2(I),I=1,5),KSTAG
PRINT 555
555 FORMAT (25H --- DATA ON TAPE 13 ---/)

```

APPENDIX A - Continued

```

C      STOP 422
560 C      PICKUP DATA ON TAPE 13
C      STOP 422
C      CONTINUE
C      IX=IX+1
C
C      CALINTH, MODIFIED RUNGE-KUTTA
C      CALL CALINTH (VAR,DER,ELE1,ELE2,CJ,SPEC,N,CUVAR,ELB,CIMAX,NERR,PHM
1AX)
C
C      IF (NERR.EQ.0) GO TO 575
C      IF (NERR.EQ.1) PRINT 565, CJ,N
565 C      FORMAT (16H BAD INPUT,CJ,N=E17.8,I5)
C      IF (NERR.EQ.2) PRINT 570, ELE1,ELE2
570 C      FORMAT (1X,21HEXAMINE ELE1 AND ELE2/10(7E17.8/))
C      IF (NERR.EQ.1.OR.NERR.EQ.2) STOP 665
C
C      STOP 665
575 C      CONTINUE
C      IF (IX.EQ.1) GO TO 580
C      IF (IPSI.EQ.6.AND.IX.EQ.6) GO TO 580
C      IF (VAR(1).GE.VARI(IZTERM)) GO TO 580
C      IF (IPSI.LT.6.AND.VAR(1).GE.DELX) GO TO 580
C      KIPF=KIPF+1
C      IF (KIPF.NE.IPF) GO TO 625
C      KIPF=0
C
C      CONTINUE
580 C      IMAXP2=IMAX+2
C      SUMCI=0.
C      DO 590 ISUM=3,IMAXP2
C      IF (VAR(ISUM).LT.0.) NEG=-1
C      IF (VAR(ISUM).LT.0.) PRINT 595
585 C      FORMAT (/5X,21H-----NEGATIVE CI-----/)
590 C      SUMCI=SUMCI+VAR(ISUM)
C      DO 595 ICM=1,IMAX
C
C      PRINT ANSWERS
595 C      CM(ICM)=VAR(ICM+2)*MU/MUI(ICM)
C      PRINT 600, IPSI,IX,XVAR,H,MU,PFTL,RHC,U,T,E,SPEC,SUMCI
600 C      FORMAT (2X12.15,8X,2HX=D15.8,7X,2HH=D15.8,6X,3HMU=E15.8,7X,2HP=E15
1.8,5X,4HRHO=E15.8/17X,2HU=E15.8,7X,2HT=E15.8,7X,2HE=E15.8,6X,3HCI=
2E15.8,1X,8HSUM(CI)=E15.8)
C      PRINT 605, (VAR(I),I=3,IMAXP2)
605 C      FORMAT (10X,9H CI( 1)=D15.8,9H CI( 2)=D15.8,9H CI( 3)=D15.8,9H
1 CI( 4)=D15.8,9H CI( 5)=D15.8/10X,9H CI( 6)=D15.8,9H CI( 7)=D15.
2.8,9H CI( 8)=D15.8,9H CI( 9)=D15.8,9H CI(10)=D15.8/10X,9H CI(1
31)=D15.8,9H CI(12)=D15.8,9H CI(13)=D15.8,9H CI(14)=D15.8,9H CI
4(15)=D15.8/10X,9H CI(16)=D15.8,9H CI(17)=D15.8,9H CI(18)=D15.8,
59H CI(19)=D15.8,9H CI(20)=D15.8/10X,9H CI(21)=D15.8,9H CI(22)=
5D15.8,9H CI(23)=D15.8,9H CI(24)=D15.8,9H CI(25)=D15.8)
C      PRINT 610, (CM(I),I=1,IMAX)
610 C      FORMAT (10X,9H CM( 1)=E15.8,9H CM( 2)=E15.8,9H CM( 3)=E15.8,9H
1 CM( 4)=E15.8,9H CM( 5)=E15.8/10X,9H CM( 6)=E15.8,9H CM( 7)=E15
2.8,9H CM( 8)=E15.8,9H CM( 9)=E15.8,9H CM(10)=E15.8/10X,9H CM(1
31)=E15.8,9H CM(12)=E15.8,9H CM(13)=E15.8,9H CM(14)=E15.8,9H CM
4(15)=E15.8/10X,9H CM(16)=E15.8,9H CM(17)=E15.8,9H CM(18)=E15.8,
59H CM(19)=E15.8,9H CM(20)=E15.8/10X,9H CM(21)=E15.8,9H CM(22)=
6E15.8,9H CM(23)=E15.8,9H CM(24)=E15.8,9H CM(25)=E15.8)
C      IMAXL=2+IMAX+IMAX
C      IMAXP3=2+IMAX+1
C      PRINT 615, (VAR(I),I=IMAXP3,IMAXL)
615 C      FORMAT (10X,9H EVI( 1)=D15.8,9H EVI( 2)=D15.8,9H EVI( 3)=D15.8,9H
1 EVI( 4)=D15.8,9H EVI( 5)=D15.8/10X,9H EVI( 6)=D15.8,9H EVI( 7)=D15
2.8,9H EVI( 8)=D15.8,9H EVI( 9)=D15.8,9H EVI(10)=D15.8/10X,9H EVI(1
31)=D15.8,9H EVI(12)=D15.8,9H EVI(13)=D15.8,9H EVI(14)=D15.8,9H EVI
4(15)=D15.8/10X,9H EVI(16)=D15.8,9H EVI(17)=D15.8,9H EVI(18)=D15.8,

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APPENDIX A - Continued

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59H EVI(19)=D15.8,9H EVI(20)=D15.8/10X,9H EVI(21)=D15.8,9H EVI(22)=
6D15.8,9H EVI(23)=D15.8,9H EVI(24)=D15.8,9H EVI(25)=D15.8)
PRINT 620
620 FORMAT (/)
C
C IF (IBUG(11).EQ.0) IBUG(11)=1
625 CONTINUE
IF (NEG.EQ.-1) PRINT 630
630 FORMAT (31H A NEGATIVE CONCENTRATION,CI)
IF (NEG.EQ.-1) STOP 670
C
C STOP 670
C
C WHEN IPSI=6, DELX AND STAGNATION STREAMLINES WILL BE COMPUTED
C
C IUNEG = 1 IF U**2 NEG. IN BASIC
IF (IUNEG.EQ.1) GO TO 735
IF (IPSI.LT.6.AND.VAR(1).LT.XPST(1)) GO TO 505
IF (ISTAG.EQ.1.OR.ISTAG.EQ.2) GO TO 690
ISTAG=0 UNTIL AFTER EXTRAPOLATION FOR PSI=0. STREAMLINE
ISTAG=1 FOR PSI =0.0 STREAMLINE
ISTAG=2 FOR DELX STREAMLINE AND THEREAFTER
C
635 CONTINUE
IG=IG+1
IGC=0
IGE=IMAX+2
PSIG(IG)=PSIS
DO 640 IG1=3,IMAXP2
IGC=IGC+1
CIG(IGC,IG)=VAR(IG1)
IGE=IGE+1
EIG(IGC,IG)=VAR(IGE)
640 CONTINUE
C
EG(IG)=E
TG(IG)=T
HG(IG)=H
IF (IPSI.LT.6) PRINT 725
IF (IPSI.LT.6) GO TO 730
C
C IPSI=6 STAGNATION STREAMLINE
C AT DELX EXTRAPOLATE FOR PSI=0. VALUES
PSI=0.
MG=1
CALL FTLUP (PSI,E,MG,IG,PSIG,EG)
CALL FTLUP (PSI,T,MG,IG,PSIG,TG)
CALL FTLUP (PSI,H,MG,IG,PSIG,HG)
C
DO 650 IG2=1,IMAX
DO 645 IG1=1,6
CIT(IG1)=CIG(IG2,IG1)
EIT(IG1)=EIG(IG2,IG1)
CALL FTLUP (PSI,CI(IG2),MG,IG,PSIG,CIT)
IF (CI(IG2).LT.0.0) CI(IG2)=0.00000001
CALL FTLUP (PSI,EVI(IG2),MG,IG,PSIG,EIT)
I3=2+IMAX+IG2
PRINT 646,IG,I3,CIT,CI(IG2),EIT,EVI(IG2),PSIG
646 FORMAT(2I5/(7E17.8))
650 VAR(2+IMAX+IG2)=EVI(IG2)
DO 655 IG1=1,6
CALL RECIN (10,1,I3,RECIN,X,ZS,RS,RC,COST,SINT)
655 CONTINUE
C INITIALIZE FOR PSI=0. STREAMLINE
CJ=XI
SPEC=0.0

```

APPENDIX A - Continued

```

II=0
KEYINT=0
IX=0
SUM=0
DO 660 I=1,IMAX
SUM=SUM+CI(I)/MUI(I)
IF (EVI(I).EQ.0.) TVI(I)=0.
IF (EVI(I).EQ.0.) GO TO 660
XL=((DGNI(I)*R*THETA(I))/(MUI(I)*EVI(I))+1.0)
ALN=ALOG(XL)
TVI(I)=THETA(I)/ALN
660 CONTINUE
PRINT 661,(EVI(I),TVI(I),I=1,IMAX)
661 FORMAT(5X,D17.8,E17.8)
C
U=SQRT(2.0*(HSTAG-H))
C
VAR(1)=DELX
C COMPUTE P AND DPDX AT IPSI=6
PRINT 665
665 FORMAT(24H PSI=0.000 STREAMLINE--)
P(6)=PS+US/(RC*RS)*(-PSIS)
RHO=P(6)/(H-E)
DO 670 I=7,IZTERM
CALL RECIN (11,1,IRECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
670 P(I)=PS+US/(RC*RS)*(-PSIS)
REWIND 10
REWIND 11
MG=1
NPG=IZTERM-5
DO 675 I=7,IZTERM
LG=I-6
675 DPDX(I)=DIF(LG,MG,NPG,VARI(6),P(6))
DO 680 I=1,5
CALL RECIN (11,1,IRECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
680 CONTINUE
ISTAG=1
PSIS=0.
CALL SECOND (CHECKT)
PRINT 685,CHECKT
685 FORMAT(14H ----- CHECKT=E15.8,6H -----/)
PRINT 686,(EVI(I),I=1,IMAX)
686 FORMAT(7D17.8)
GO TO 500
C
690 CONTINUE
C
C AT EACH X WHERE PHYSICAL SPACE CALCULATIONS ARE DESIRED SAVE
C 1./(RHO*U) ON EACH STREAMLINE
C
IF (VAR(1).LT.XPST(LPS2)) GO TO 720
IF (VAR(1).GT.XPST(LPS2)) GO TO 705
C VAR(1) = XPST(LPS2)
RHOURL=1./(RHO*U)
IF (IBUG(13).NE.0) GO TO 700
PRINT 695,IPSI,RHOURL
695 FORMAT(7H IPSI=I3.9H RHOURL=E15.8)
700 CONTINUE
CALL REOUT (12,1,0,IPSI,RHOURL,VAR(1),PSIS)
GO TO 715
705 YPSIS=PREPSIS+(XPST(LPS2)-PREX)*((PSIS-PREPSIS)/(VAR(1)-PREX))
RHOURL=PRERU+(XPST(LPS2)-PREX)*((RHO*U-PRERU)/(VAR(1)-PREX))
RHOURL=1./RHOURL

```

APPENDIX A - Continued

```

CALL RECOUT (12,1,0,IPSI,RHOURT,XPST(LPS2),YPSIS)
IF (IBUG(13).NE.0) GO TO 715
PRINT 695, IPSI,RHOURT
PRINT 710, LPS1,LPS2,VAR(1),XPST(LPS2),PREPSIS,PSIS,PRERU,PREX
710  FORMAT (12H LPS1,LPS2=2I4,33H X,XPST,PREPSIS,PSIS,PRERU,PREX=/D1
17.8,5E17.8)
715  CONTINUE
LPS2=LPS2+1
KSTAG=KSTAG+1
720  CONTINUE
PREX=VAR(1)
PRERU=RHO*U
PREPSIS=PSIS
IF (VAR(1).LT.VARI(IZTERM)) GO TO 505
C      END OF A STREAMLINE
PRINT 725
725  FORMAT (/20H XXXXXXXXXXXXXXXXXXXX/)
IF (IPSI.EQ.6.AND.ISTAG.EQ.1) GO TO 425
730  CONTINUE
GO TO 420

C
C      COMPUTE PHYSICAL SPACE VALUES
C
735  CONTINUE
CALL SECOND (CHECKT)
PRINT 695, CHECKT
REWIND 8
REWIND 9
REWIND 10
REWIND 11
PRINT 740, KSTAG
740  FORMAT(37H BEGIN PHYSICAL SPACE CALCULATIONS AT,15,10H LOCATIONS/)
C
DO 840 LPS=1,NXPST
REWIND 12
IK=0
745  CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
IF (ENDFILE 10) 845,750
750  CONTINUE
IF (IBUG(13).NE.0) GO TO 760
PRINT 755, LPS,X,XPST(LPS)
FORMAT (18H LPS,X,XPST(LPS) 15,2E30,15/)
755  CONTINUE
IF (ABS(X-XPST(LPS)).GT.1.0E-8) GO TO 745
IF (IBUG(13).NE.0) GO TO 765
760  PRINT 755, LPS,X,XPST(LPS)
C
765  CONTINUE
DO 780 IPS=1,KSTAG
CALL RECIN (12,1,IRECIN,IPSI,RHOURT,VAR(1),PSIS)
VARMX=VAR(1)-XPST(LPS)
IF (ABS(VARMX).GT.1.0E-8) GO TO 780
IK=IK+1
IF (IK.GT.200) PRINT 770, IK
770  FORMAT (1X,50HIK.GT.200, CHANGE DIMENSION OF RUT AND PSISTG, IK=,I
13)
RUT(IK)=RHOURT
PSISTG(IK)=PSIS
IF (IBUG(13).NE.0) GO TO 780
PRINT 775, PSIS,RHOURT
775  FORMAT (14H PSIS,RHOURT=2E17.8)
780  CONTINUE
C      FIND SMALLEST DELTA PSI

```

APPENDIX A - Continued

```

SMALL=200.
DO 785 I=2,IK
IF (PSISTG(I)-PSISTG(I-1)).LT.SMALL) SMALL=PSISTG(I)-PSISTG(I-1)
785 CONTINUE
XDEL=PSISTG(IK)/SMALL
C TRUNCATE
L=INT(XDEL+1.)
C REMAINDERING M=0 FOR EVEN, M=1 FOR ODD
M=MOD(L,2)
C MAKE L EVEN
IF (M.NE.0) L=L+1
C FIND INTEGRAL 1./(RHO*U) DELTA PSI FROM BODY TO SHOCK
C SIMPSON-S RULE L INCREMENTS, L+1 POINTS
FL=L
DPSIS=PSISTG(IK)/FL
PSII=0.
RB=RUT(1)+RUT(IK)
LM1=L-1
IF (IBUG(13).NE.0) GO TO 795
PRINT 790, L,M,SMALL,XDEL,DPSIS,RB
790 FORMAT (25H L,M,SMALL,XDEL,DPSIS,RB/2I5,4E17.8)
795 CONTINUE
DO 800 I=2,L,2
PSII=PSII+DPSIS
CALL FTLUP (PSII,RU1,1,IK,PSISTG,RUT)
IF (I.EQ.L) RB=RB+4.*RU1
IF (I.EQ.L) GO TO 800
PSII=PSII+DPSIS
CALL FTLUP (PSII,RU2,1,IK,PSISTG,RUT)
RB=RB+4.*RU1+2.*RU2
800 CONTINUE
C
RB=RB*DPSIS/3.
IF (IBUG(13).NE.0) GO TO 810
PRINT 805, RB,RS,COST,RB,SINT
805 FORMAT (21H RB,RS,COST,RB,SINT=5E17.8)
810 CONTINUE
ARR=SQRT(RS**2-2.*COST*RB)
YI=(RS-ARR)/COST
ZE=ZS+YI*SINT
PRINT 815, X,ARR,YI,ZE,PSISTG(1)
815 FORMAT (3H X=E15.8,5H R=E15.8,5H Y=E15.8,5H Z=E15.8,7H PSI
1=E15.8)
C
DO 830 I=2,IK,1
DPSI=PSISTG(I)-PSISTG(I-1)
C TRAPEZOIDAL RULE
TR=(DPSI/2.)*(RUT(I)+RUT(I-1))
RB=RB-TR
IF (IBUG(13).NE.0) GO TO 825
PRINT 820, TR,RB
820 FORMAT (5HTR,RB,2E17.8)
825 CONTINUE
ARR=SQRT(RS**2-2.*COST*RB)
YI=(RS-ARR)/COST
ZE=ZS+YI*SINT
PRINT 835, X,ARR,YI,ZE,PSISTG(I)
830 CONTINUE
PRINT 835
835 FORMAT (/)
C
840 CONTINUE
845 CONTINUE
PRINT 850
850 FORMAT (29H END THIS CASE, HALLELUJAH)

```

APPENDIX A - Continued

```

STOP
END
SUBROUTINE BASIC
C BASIC CALLED BY CALINTH TO EVALUATE DERIVATIVES H DOT,
C SUB I DOT AND EV SUB I DOT
C DERIVATIVES START IN DER(1)
C
COMMON M,IX,IMAX,IPSI,IBUG(15)
COMMON P( 500),OPDX( 500),VARI( 500)
COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
1 LI(25)
COMMON R,MUINF,DELTA,LAMSQ,OMEGSQ,OMEGA,MU,T,U
COMMON EPSIIL(20,25),GIL(20,25)
COMMON VAR(52),CUVAR(52),DER(51)
C
COMMON ZS,RS,RC,SINT,COST,PS,US,PSIS
COMMON MJ(50),EJ(50),AJ(50),BJ(50)
COMMON TVI(25),NI(25),DGENI(25)
COMMON NUIJ(26,50),AIJ(25,50),NUPIJ(25,50)
COMMON SIGIK(25,25),ALPIK(25,25),BETAIK(25,25)
C
COMMON /LAB2/ DELX,ZSTERM,IZTERM
COMMON /LAB3/ EINF,PINF,RHOINF,VINF,E,JMAX,KEYINT,RHO,HSTAG
COMMON /LAB4/ PFTL,KITR1,EITR1
COMMON /LAB5/ IUNEG
COMMON /LAB7/ ITNEG,IEXP
C
DOUBLE PRECISION VAR
C
DIMENSION PHI(50),KJ(50),SJ(50)
DIMENSION CI(25),EVI(25),DCIDX(25),DEVIDX(25),EVIBAR(25)
C
EQUIVALENCE (CUVAR(2),H),(CUVAR(3),CI(1))
EQUIVALENCE (DER(1),DHDX),(DER(2),DCIDX(1))
C
REAL KJ,LAMSQ,MU,MUI,MUINF,NI,NUIJ,NUPIJ
C
DER(1)=DHDX          MUST BE DHDX AS H MAY BE + OR -
DER(2)= DCIDX(1)
C
-
C
DER(1+IMAX      )=DCIDX(IMAX)
C
DER(1+IMAX+1    )=DEVIDX(1)
C
DER(1+IMAX+IMAX)=DEVIDX(IMAX)
C
CUVAR(1) = X
C
CUVAR(2) = H,ENTHALPY - IT MUST BE H WHICH MAY BE + OR -
C
CUVAR(3) = CI(1)
C
-
C
CUVAR(2+IMAX      )=CI(IMAX)
C
CUVAR(2+IMAX+1    )=EVI(1)
C
CUVAR(2+IMAX+IMAX)=EVI(IMAX)
C
EXTERNAL FOFE
C
KEYINT=1 AT END OF 1ST INTERVAL
IF (ITNEG.EQ.1.OR.IEXP.EQ.1) RETURN
IF (M.NE.0) GO TO 10
DO 5 I=1,IMAX
J1=I+IMAX+2
5 CUVAR(J1)=VAR(J1)
10 CONTINUE
C
INTERPOLATE FOR P ACROSS INTEGRATION INTERVAL
DO 15 I=1,IMAX
15 EVI(I)=CUVAR(2+IMAX+I)
MFTL=1
NFTL=IZTERM-IPSI+1
CALL FTLUP (CUVAR(1),PFTL,MFTL,NFTL,VARI(IPSI),P(IPSI))

```

APPENDIX A - Continued

```

C      INTERPOLATE FOR DPDX
CALL FTLUP (CUVAR(1),DPFTL,MFTL,NFTL,VARI(IPSI),DPDX(IPSI))
IF (IBUG(10).NE.0) GO TO 30
PRINT 20, E,PFTL,P(IPSI),P(IPSI+1),CUVAR(1),DPFTL,DPDX(IPSI)
20  FORMAT (25H E,PFTL,P(IT ),P(IT +1/7E17.8)
PRINT 25, (CI(IU),IU=1,IMAX),(EVI(IU),IU=1,IMAX)
25  FORMAT (5E18.8)
30  CONTINUE
IF (KEYINT.EQ.0) GO TO 95
SUM=0.

C      COMPUTE TVI
DO 45 I=1,IMAX
C      USE SHOCK VALUES FOR INITIAL COMPUTATION ON EACH STREAMLINE
SUM=SUM+CI(I)/MUI(I)
IF (EVI(I).EQ.0.) TVI(I)=0.
IF (EVI(I).EQ.0.) GO TO 35
XL=((DGENI(I)*R*THETA(I))/(MUI(I)*EVI(I))+1.0)
ALN=ALOG(XL)
TVI(I)=THETA(I)/ALN
35  CONTINUE
IF (IBUG(10).GT.0) GO TO 45
PRINT 40, I,DGENI(I),R,THETA(I),MUI(I),EVI(I),XL,ALN,TVI(I)
40  FORMAT (26H I,DGENI,R,THETA,MUI,EVI/I5.6E17.8/11H XL,ALN,TVI/3E1
18.8/)
45  CONTINUE
MU=1.0/SUM

C
U2=2.0*(HSTAG-H)

C
IF (U2.LT.0.) PRINT 50, H
50  FORMAT (32H USQUARED IS NEG. IN DERSUB, H=E15.8.29H  END STREAML
1INE INTEGRATION)
IF (U2.LT.0.) IUNEG=1
IF (U2.LT.0.) RETURN
U=SQRT(U2)

C      ITERATE FOR E
KCODE=0
55  CONTINUE
KITR1=0
DELTE=100000.
E1=.00001
E2=.001
MAXI=10

C
CALL ITR1 (E,DELTE,FOFE,E1,E2,MAXI,ICODE)
C      C5.002 LF-ITR1
IF (ICODE.EQ.0) GO TO 75
IF (ICODE.EQ.1) PRINT 60
60  FORMAT (38H FOFE, MAXIMUM ITERATION EXCEEDED ***/)
IF (ICODE.EQ.2) PRINT 65
65  FORMAT (25H FOFE, DERIVATIVE=0 ****/)
PRINT 70, ICODE
70  FORMAT (13H ITR1,ICODE=I2)
IF (ICODE.NE.1) STOP 66

C
C      WHEN ICODE=1, TRY A NEW STARTING E. DO THIS 2 TIMES
IF (KCODE.EQ.3) STOP 66

C
E=EITR1
KCODE=KCODE+1
GO TO 55
75  CONTINUE
IF (IEXP.NE.1) GO TO 65
E=EITR1

```

APPENDIX A - Continued

```

KCODE=1+KCODE
IEXP=0
PRINT 80, KCODE
80  FORMAT (8H KCODE=I2)
    IF (KCODE.EQ.1) GO TO 55
    IF (KCODE.GT.2) RETURN
    E=H-0.00001*H
    GO TO 55
85  CONTINUE
    RHO=PFTL/(H-E)
    T=(PFTL*MU)/(RHO*R)
    IF (T.GT.0.0) GO TO 95
    PRINT 90, T,RHO,PFTL,H,E,MU
90  FORMAT (14H T NEGATIVE =E15.8,2X,4HRHO=E15.8,2X,5HPFTL=E15.8,2X,2
1HH=E15.8,2X,2HE=E15.8,2X,3HMU=E15.8)
    E=H-0.00001*H
    ITNEG=1
    RETURN
C
95  CONTINUE
    KEYINT=1
    IF (IBUG(9).NE.0) GO TO 110
    PRINT 100, IX,IPSI,RHO,T,MU,U,H
100  FORMAT (16H IX,IPSI,RHO,T=2I4,4E17.8,E17.8/)
    PRINT 105, E
105  FORMAT (4H E=E18.8/)
110  CONTINUE
C      COMPUTE DCIDX AND DEVIDX FOR EACH SPECIE
DO 210 I=1,IMAX
C      FOR EACH REACTION
    DCIDX(I)=0.
    DO 190 J=1,JMAX
C      SELECTED SPECIE FOR THIS REACTION
        II=MJ(J)
        IF (M.EQ.0) GO TO 115
        IF (FI(II).NE.0.) GO TO 120
115  PHI(J)=1.0
        GO TO 125
120  CONTINUE
        TEM=EXP(THETA1(II)/TVI(II))
        TEM1=EXP(THETA1(II)/T)
        TEM2=EXP(-NI(II)*(THETA1(II)/TVI(II)-THETA1(II)/T))
        TEM3=EXP(THETA1(II)/TVI(II)-THETA1(II)/T)
        IF (TEM3.EQ.1.0) PHI(J)=1.0
        IF (TEM3.EQ.1.0) GO TO 125
C      PHI=COUPLING COEFFICIENT, VIBRATION AND DISSOCIATION INTERACTION
        PHI(J)=((1.0-TEM2)/(TEM3-1.0)*(TEM-1.0)/(TEM1-1.0))/NI(II)
125  TEM4=EXP(-EJ(J)/T)
C      KJ = RATE CONSTANT
        KJ(J)=AJ(J)*T**BJ(J)*TEM4
        IF (NUIJ(IMAX+1,J).EQ.0.) SJ(J)=1.0
        IF (NUIJ(IMAX+1,J).EQ.0.) GO TO 140
        SUM=0.
        DO 135 ISUM=1,IMAX
C
            SUM=SUM+AIIJ(ISUM,J)*CI(ISUM)/MUI(ISUM)
            IF (IBUG(7).NE.0) GO TO 135
            PRINT 130, I,J,ISUM,SUM,AIIJ(ISUM,J),CI(ISUM),MUI(ISUM)
130  FORMAT (25H I,J,ISUM,SUM,AIIJ,CI,MUI/3I5,5E17.8/)
C
135  CONTINUE
        SJ(J)=RHO*SUM
140  CONTINUE
        IF (IBUG(7).NE.0) GO TO 150
C
80

```

APPENDIX A - Continued

```

PRINT 145, I, J, FI(I), PHI(J), TEM, TEM1, TEM2, TEM3, TEM4, AJ(J), BJ(J), T
1, KJ(J), SUM, RHO, SJ(J)
145  FORMAT (26H I, J, FI, PHI, TEM, TEM1, TEM2/2I5, 5E18.8/22H TEM3, TEM4, AJ
1, BJ, T, KJ/6E18.8/12H SUM, RHO, SJ/3E18.8/)
C
150  CONTINUE
PROD=1.0
DO 180 IPROD=1, IMAX
IF (NUIJ(IPROD, J).EQ.0.0) GO TO 170
TEM=RHO*CI(IPROD)/MUI(IPROD)
IF (TEM.GE.0.) GO TO 165
C      LET PROBLEM COMPUTE THRU DERSUB WHEN CI NEG,
C      MAKE DECISION IN MAIN ABOUT ACCEPTING NEG CI
ABW=AMOD(NUIJ(IPROD, J), 2.0)
IF (IBUG(8).NE.0) GO TO 160
IF (TEM.LT.0.) PRINT 155, I, J, IX, IPROD, TEM, RHO, MUI(IPROD), NUIJ(IPR
100, J), CI(IPROD), PROD, ABW
155  FORMAT (2X, 32H I, J, IX, IPROD, TEM, RHO, MUI, NUIJ, CI/4I3, 7E17.8)
160  CONTINUE
C      ABW=0.0 FOR EVEN NUIJ, ABW=1.0 FOR ODD NUIJ
IF (ABW.EQ.0.0) PROD=PROD*(-TEM)**NUIJ(IPROD, J)
IF (ABW.EQ.1.0) PROD=-1.0*PROD*(-TEM)**NUIJ(IPROD, J)
GO TO 170
165  CONTINUE
PROD=PROD*TEM**NUIJ(IPROD, J)
C
170  CONTINUE
IF (IBUG(8).NE.0) GO TO 180
IF (IX.LT.3) GO TO 180
PRINT 175, I, J, IPROD, TEM, PROD, RHO, CI(IPROD), NUIJ(IPROD, J)
175  FORMAT (48H I, J, IPROD, TEM, PROD, RHO, CI(IPROD), NUIJ(IPROD, J)/3I5, 6E
117.8/)
180  CONTINUE
DCIJDX=PHI(J)*KJ(J)*SJ(J)*(MUI(I)/(RHO*U))*(NUPIJ(I, J)-NUIJ(I, J))*
1 PROD
C
C      DCIDX = RATE OF APPEARANCE AND DISAPPEARANCE OF CONCENTRATION
C      OF SPECIE
C      DCIDX(I)=DCIDX(I)+DCIJDX
C
IF (IBUG(8).NE.0) GO TO 190
PRINT 185, I, J, DCIJDX, PHI(J), KJ(J), SJ(J), MUI(I), RHO, U, NUPIJ(I, J), N
1 UIJ(I, J), PROD, DCIDX(I)
185  FORMAT (25H I, J, DCIJDX, PHI, KJ, SJ, MUI/2I5, 5E18.8/29H RHO, U, NUPIJ, N
1 UIJ, PROD, DCIDX/6E18.8/)
190  CONTINUE
TEM=EXP(THETA(I)/T)
TEM1=(FI(I)*DGENI(I)*R*THETA(I))/MUI(I)
EVIBAR(I)=TEM1/(TEM-1.0)
IF (M.NE.0) GO TO 195
VAR(I+IMAX+2)=EVIBAR(I)
DEVIDX(I)=0.
GO TO 210
195  CONTINUE
TAUSUM=0.
IF (FI(I).EQ.0.) GO TO 210
DO 205 K=1, IMAX
TEM3=EXP(-THETA(I)/T)
TEM4=EXP(SIGIK(K, I)*T**(-1./3.))
TEM5=(FI(I)*ALPIK(K, I))/PFTL
TAUIK=TEM5*(T**BETA(K, I)*TEM4)/(1.0-TEM3)
TEM6=CI(K)*(EVIBAR(I)-EV(I))
TAUSUM=TAUSUM+TEM6/(TAUIK*U)
C

```

APPENDIX A - Continued

```

      IF (IBUG(9).NE.0) GO TO 205
      PRINT 200, I,K,TEM3,TEM4,TEM5,TAUIK,TAUSUM,SIGIK(K,I),ALPIK(K,I),B
1  ETAIK(K,I),U,EVI(I),EVIBAR(I),TEM,TEM1,TEM2,TEM6,TEM6
200  FORMAT (33H I,K,TEM3,TEM4,TEM5,TAUIK,TAUSUM/215.5E18.8/33H SIGIK
1  ,ALPIK,BETAIK,U,EVI,EVIBAR/6E17.8/22H TEM,TEM1,TEM2,TEM6 /4E18.8
2  ,022/)
205  CONTINUE
C
C      DEVIDX = EQUILIBRIUM VIBRATIONAL ENERGY
      DEVIDX(I)=TAUSUM
      DER(1+IMAX+I)=DEVIDX(I)
210  CONTINUE
C      COMPUTE DHDX
      DHDX=DPFTL/RHO
      IF (IBUG(10).NE.0) RETURN
      PRINT 215, DEVIDX(I)
215  FORMAT (9H DEVIDX=E22.14)
      PRINT 220, DPFTL,DHDX
220  FORMAT (12H DPDX,DHDX=2E18.8,16H          END BASIC////)
      RETURN
      END
      FUNCTION FOFE(DUM)
C
C      CALLED BY ITR1 IN EASIC TO EVALUATE E
C
      COMMON M,IX,IMAX,IPSI,IBUG(15)
      COMMON P( 500),DPEX( 500),VARI( 500)
      COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
1  LI(25)
      COMMON R,MUINF,DELTA,LAMSQ,OMEGSQ,OMEGA,MU,T,U
      COMMON EPSIIL(20,20),GIL(20,20)
      COMMON VAR(52),CUVAR(52),DER(51)
C
      COMMON ZS,RS,RC,SINT,COST,PS,US,PSIS
      COMMON MJ(50),EJ(50),AJ(50),BJ(50)
      COMMON TVI(25),NI(25),DGENI(25)
      COMMON NUIJ(21,30),AIJ(20,30),NUIPJ(20,30)
C
      COMMON /LAB4/ PFTL,KITR1,EITR1
      COMMON /LAB7/ ITNEG,IEXP
C
      DOUBLE PRECISION VAR
C
      DIMENSION CI(25)
C
      EQUIVALENCE (CUVAR(3),CI(1)),(CUVAR( 2),H)
C
      REAL MUI,LAMSQ,MUINF,MU
C
      IF(ITNEG.EQ.1.OR.IEXP.EQ.1) RETURN
      KITR1=KITR1+1
      IF (KITR1.EQ.3) EITR1=DUM
      PORHO=H-DUM
      E=0
      EDUM=DUM
      T=PORHO*MU/R
      IF (IBUG(11).NE.0) GO TO 10
      PRINT 5, EDUM,MU,T,RHO,PFTL,H
5  FORMAT(1X,5HEDUM=E15.8,2X,3HMU=E15.8,2X,2HT=E15.8,2X,4HRHO=E15.8,
1  2X,5HPFTL=E15.8,2X,2HH=E15.8)
10  CONTINUE
C
      DO 35 I=1,IMAX
      IF (TVI(I).EQ.0.) TEM1=(1.5*R*T)/MUI(I)+(FI(I)*R*T)/MUI(I)
      IF (TVI(I).EQ.0.) GO TO 15

```

APPENDIX A - Continued

```

TEM=EXP(THETAI(I)/TVI(I))
TEM1=(1.5*R*T)/MUI(I)+(FI(I)*R*T)/MUI(I)+(FI(I)*R*THETAI(I))/(MUI(
11)*(TEM-1.0))
15 CONTINUE
SUMG=0.
SUMGE=0.
C
LII=LI(I)
DO 25 L=1,LII
TEM3=-EPSIIL(L,I)/T
IF(TEM3.LT.741.67) GO TO 42
PRINT 41, TEM3,EPSIIL(L,I),T,EDUM,L,I,H,MU,KITR1
41 FORMAT(56H EXP(TEM3), TEM3.GT.741.67, TEM3,EPSIIL(L,I),T,EDUM,L,I=
1 /4E17.8,2I5,13H F,MU,KITR1=2E17.8,15)
IEXP=1
C SET IEXP=1 TO TRIGGER REDUCTION IN COMPUTING INTERVAL
C AND A NEW E ESTIMATE
RETURN
42 TEM2=EXP(TEM3)
SUMG=SUMG+GIL(L,I)*TEM2
SUMGE=SUMGE+GIL(L,I)*EPSIIL(L,I)*TEM2
IF(SUMGE.GT.10.E300) IBUG(11)=0
C
IF( (IBUG(11)).NE.0) GO TO 25
PRINT 20, I,L,TEM2,EPSIIL(L,I),T,SUMG,GIL(L,I),SUMGE
20 FORMAT(34H I,L,TEM2,EPSIIL,T,SUMG,GIL,SUMGE/2I5,6E18.8/)
25 CONTINUE
IF(SUMGE.LT.10.E300) GO TO 26
PRINT 27
C
27 FORMAT( 56H IN FCFE,SUMGE.GT.10.E300, SET IEXP=1 TO REDUCE INTERVA
1L/)
C
IBUG(11)=1
IEXP=1
RETURN
26 CONTINUE
EI=TEM1+R/MUI(I)*(SUMGE/SUMG)+DELHI(I)/MUI(I)
E=E+EI*CI(I)
IF (IBUG(11)).NE.0) GO TO 35
PRINT 30, I,L,IX,IPSI,PORHO,E,EDUM,H,RHO,T,TEM,TEM1,SUMG,SUMGE,EI,
1E
10 FORMAT(32H I,L,IX,IPSI,PORHO,E,EDUM,H,RHO/4I4,6E18.8/23H T,TEM,
ITEM1,SUMG,SUMGE/7E18.8//)
15 CONTINUE
FOFE=E
IF (E.GT.H) PRINT 4C, E,H
40 FORMAT(26H IN ITR1-FOFE, E.GT.H, E=E15.8, 6H H=E15.8,
1 5X, 17H REDUCE INTERVAL)
IF(E.GT.H) ITNEG=1
;
RETURN
END
FUNCTION FOFTS(CUM)
C
C CALLED BY ITR1 IN MAIN PROGRAM TO EVALUATE TS
C
COMMON M,IX,IMAX,IPSI,IBUG(15)
COMMON P( 500),DPDX( 500),VARI( 500)
COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
1 LI(25)
COMMON R,MUINF,DELTA,LAMSG,OMEGSQ,OMEGA,MU,T,U
COMMON EPSIIL(20,20),GIL(20,20)
COMMON VAR(52),CUVAR(52),DER(51)
C

```

APPENDIX A - Continued

```

DOUBLE PRECISION VAR
C
DIMENSION CI(25)
C
EQUIVALENCE (CUVAR(3),CI(1))
C
REAL MUI,LAM SQ,MUINF,MU
C
ES=0
DO 25 I=1,IMAX
  IF (M.EQ.1) EVIS=EVIINF(I)
  IF (M.EQ.1) GO TO 5
C
  TEM=EXP(THETAI(I)/DUM)
C
  EVIS=(R*THETAI(I))/(MUI(I)*(TEM-1.0))*FI(I)
5
  SUMG=0
  SUMGE=0
C
  LII=LI(I)
  DO 10 L=1,LII
    TEM1=EXP(-EPSIIL(L,I)/DUM)
    SUMG=SUMG+TEM1*GIL(L,I)
10
    SUMGE=SUMGE+TEM1*GIL(L,I)*EPSIIL(L,I)
    EEIS=(R/MUI(I))*(SUMGE/SUMG)
    EIS=(1.5*R*DUM)/MUI(I)+(FI(I)*R*DUM)/MUI(I)+EVIS+EEIS+DELHI(I)/MUI
    1(I)
    ES=ES+EIS*CIINF(I)
    IF (IBUG(4).NE.0) GO TO 20
    T=DUM
15
    PRINT 15, IX,I,M,EVIS,TEM,T,SUMG,SUMGE,TEM1,EEIS,EIS,ES,CIINF(I)
    FORMAT (32H IX,I,M,EVIS,TEM,DUM,SUMG,SUMGE/315,5E18.8/30H TEM1,E
    1EIS,EIS(I),ES,CIINF(I)/5E18.8/)
C
20
  CONTINUE
25
  CONTINUE
C
  FAC=SQRT(OMEGSQ-2.*LAM SQ*(DELTA-ES))
  FIN=(2.*MUINF*(DELTA-ES)*FAC)/(R*(OMEGA+FAC))
  FOFTS=FIN
  IF (IBUG(4).NE.0) RETURN
  PRINT 30, CMEGSQ,LAM SQ,DELTA,ES,MUINF,FAC,R,OMEGA,FIN
30
  FORMAT (44H OMEGSQ,LAM SQ,DELTA,ES,MUINF,FAC,R,OMEGA,FIN/2(5E18.8/
  1)
  RETURN
  END
  SUBROUTINE FDP CX
C
  TO COMPUTE P AND CFCX
C
  AND SAVE ON TAPES 9 AND 8
C
  COMMON M,IX,IMAX,IPSI,IBUG(15)
  COMMON P( 500),DPCX( 500),VARI( 500)
  COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
  1
  LI(25)
  COMMON R,MUINF,DELTA,LAM SQ,CMEGSQ,CMEGA,MU,T,U
  COMMON EPSIIL(20,20),GIL(20,20)
  COMMON VAR(52),CUVAR(52),DER(51)
C
  COMMON ZS,RS,RC,SINT,COST,PS,US,PSIS
  COMMON MJ(50),EJ(50),AJ(50),BJ(50)
  COMMON TVI(25),NI(25),DGENI(25)
  COMMON NUIJ(21,20),AIJ(20,30),NUPIJ(20,30)
  COMMON SIGIK(20,20),ALPIK(20,20),BETAIK(20,20)
  COMMON KSTAG,IMAXP2,IMAXL,N,IG,ISTAG,LPS2,LPS1,IMAXP1

```

APPENDIX A - Continued

```

COMMON X,TS,ES,RHOS,HS,RHOURT,PHMAX,CIMAX,PREPSIS,PREX,PRERU
COMMON EVIS(25),XPST(100)
C
COMMON /LAB2/ DELX,ZTERM,IZTERM
C
DOUBLE PRECISION VAR
C
                BEGIN PRESSURE DISTRIBUTION
C                FOR EACH PSI FIND RANGE OF X
C
DO 20 IPSI=1,IZTERM
DO 15 IX=1,IZTERM
  IEOF=10
  CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
  IF (EOF,10) 75,5
5  CONTINUE
  IF (IX.EQ.IPSI) XX=X
  IEOF=11
  CALL RECIN (11,1,IRECIN,IXT,TS,ES,PS,RHOS,US,PSIS,HS)
  CALL RECIN (11,2,IRECIN,EVIS,1,IMAX,1)
  IF (EOF,11) 75,10
10 CONTINUE
  IF (IXT.LT.IPSI) GO TO 15
  IF (IXT.EQ.IPSI) PSISHK=PSIS
  IF (IPSI.EQ.IX) P(IX)=PS
  IF (IPSI.EQ.IX) GO TO 15
  P(IX)=PS+US/(RC*RS)*(PSISHK-PSIS)
C
15 CONTINUE
  REWIND 10
  REWIND 11
C
  CALL RECOUNT (9,1,0,XX)
  CALL RECOUNT (9,2,0,P,IPSI,IZTERM,1)
C
20 CONTINUE
  REWIND 9
  N=1
  IEOF=9
  DO 65 IPSI=1,IZTERM
  CALL RECIN (9,1,IRECIN,X)
  CALL RECIN (9,2,IRECIN,P,IPSI,IZTERM,1)
  IF (EOF,9) 75,35
35 CONTINUE
  ITHIS=0
  DO 40 IX=IPSI,IZTERM
  IF (IX.EQ.IPSI) XT=X
  IF (IX.GT.IPSI.AND.IPSI.LT.7) XT=XT+DELX/5.
  IF (IX.GT.IPSI.AND.IPSI.GT.6) XT=XT+DELX
  IF (IX.EQ.IZTERM-1) P(IX+2)=0.0
  ITHIS=IThis+1
  VARI(IThis)=XT
40 CONTINUE
  IHERE=0
C
DO 60 IX=IPSI,IZTERM
  IF (IX.EQ.IZTERM) P(IX+1)=0.
  IF (IX.EQ.IZTERM) P(IX+2)=0.0
  IHERE=IHERE+1
C
                DIFFERENTIATE
  IF (IX.NE.IPSI) GO TO 45
  DPDX(IX)=(-3.*P(IX)+4.*P(IX+1)-P(IX+2))/(2.*DELX)
  GO TO 50
45 CONTINUE
  DPDX(IX)=(-P(IX-1)+P(IX+1))/(2.*DELX)
  IF (IX.NE.IZTERM) GO TO 50

```

APPENDIX A - Continued

```

50  DPDX(IX)=(P(IX-2)-4.*P(IX-1)+3.*P(IX))/(2.*DELX)
    CONTINUE
    IF (IBUG(1).NE.0) GO TO 60
    PRINT 55, IPSI,IX,A,DPDX(IX),P(IX)
55  FORMAT (2I5,3E18.8)
60  CONTINUE
C
    CALL RECOUT (8,2,0,DPDX,IPSI,IZTERM,1)
C
65  CONTINUE
    DO 70 IX=1,IZTERM
    IF(IX.EQ.1) VARI(1)=0.
    IF(IX.EQ.1) GO TO 70
    IF (IX.LT.7) VARI(IX)=VARI(IX-1)+DELX/5.
    IF (IX.GT.6) VARI(IX)=VARI(IX-1)+DELX
70  CONTINUE
    REWIND 9
    REWIND 8
    REWIND 10
    REWIND 11
    RETURN
75  PRINT 80, IEOF
80  FORMAT( 7H EOF 15, 13H      IN FDPDX)
    STOP 50
C
    END
    SUBROUTINE CHECK
C
C  CHECK CALLED BY CALINTH TO MAKE DECISION TO ACCEPT ANSWERS
C    IF ACCEPTABLE, SET ELB=0 AND RETURN
C    IF NOT ACCEPTABLE MODIFY SPEC AND CI. SET ELB=1.0 AND RETURN
C
    COMMON M,IX,IMAX,IPSI,IBUG(15)
    COMMON P( 500),DPDX( 500),VARI( 500)
    COMMON EVIINF(25),THETA1(25),MUI(25),FI(25),DELHI(25),CIINF(25),
1    LI(25)
    COMMON R,MUINF,DELTA,LAMSG,GMESG,OMEGA,MU,T,U
    COMMON EPSIIL(20,20),GIL(20,20)
    COMMON VAR(52),CUVAR(52),DER(51)
C
    COMMON /LAB6/ ELB,SPEC,CJ,TPREV,HPREV,HCHECK,TCHECK
    COMMON /LAB7/ ITNEG,IEXP
C
    EQUIVALENCE (CUVAR( 2),H)
C
    DOUBLE PRECISION VAR
C
    IF(IEXP.NE.1) GO TO 1
    GO TO 15
C
    REDUCE COMPUTING INTERVAL TO TRY TO AVOID EXP ERROR STOP
1  CONTINUE
    IF(ITNEG.EQ.0) GO TO 4
    IF (E.GT.H LEADS TO NEG T SOMETIMES---LETS REDUCE INTERVAL TO TRY
C    TO AVOID INSTABILITY
C
    GO TO 15
4  CONTINUE
    IMAXP1=IMAX+1
    DO 10 I=3,IMAXP1
C
        CUVAR(2)=H MAY BE NEG
    IF (CUVAR(1).LT.0.) PRINT 5, I,IX,CUVAR(1)
5  FORMAT(24H NEG CI, I,IX,CUVAR(1)=2I5,E17.8)
    IF (CUVAR(1).LT.0.) GO TO 15
10  CONTINUE
    IF (IX.LT.3) GO TO 30
    IF (IPSI.EQ.6.AND.IX.LT.8) GO TO 30
    IF(ABS(TPREV-T)/T.LT.TCHECK) GO TO 25

```

APPENDIX A - Continued

```

PRINT 11
11 FORMAT(33H CHECK-ABS(TPREV-T)/T.GE.TCHECKT)
15 CONTINUE
IF(SPEC.LT.1.0E-15) STOP 30
C
C      REDUCE INTERVAL
SPEC=SPEC/4.
CJ=SPEC
ELB=1.0
PRINT 44,SPEC,IPSI,IX,T,TPREV,H,HPREV,IEXP,ITNEG
44 FORMAT(14H REDUCED SPEC=E15.8,10H IPSI,IX=2I5,18H T,TPREV,H,HPRE
1V=4E16.7/13H IEXP,ITNEG=2I3)
ITNEG=0
IEXP=0
RETURN
25 CONTINUE
IF(ABS((HPREV-F)/H).GT.HCHECK) PRINT 42
42 FORMAT(35H CHECK,AES((HPREV-H)/H).GT.HCHECKT)
IF(ABS((HPREV-H)/H).GT.HCHECK) GO TO 15
30 CONTINUE
C      ACCEPTABLE
TPREV=T
HPREV=H
ELB=0.
RETURN
END
SUBROUTINE SHOCKG(CELX,ZSTERM,IZTERM)
SUBROUTINE SHOCKG CALLED BY MAIN
C
C      SHOCKG SUBROUTINE MUST BE SUPPLIED BY USER. IT SHOULD DEFINE THE
C      SHOCK GEOMETRY AND STORE ON TAPE 10,X,ZS,RS,RC,COST,SINT FOR EACH
C      X FROM 0.0 TO X AT ZSTERM IN INCREMENTS OF CELX/5.0 TO CELX AND
C      INCREMENTS OF CELX THEREAFTER
C      X=DISTANCE ALONG SHOCK
C      ZS=DISTANCE ALONG SHOCK AXIS OF SYMMETRY
C      RS=RADIUS OF SHOCK
C      RC=RADIUS OF CURVATURE OF SHOCK
C      COST=COS OF ANGLE OF ATTACK
C      SINT=SIN OF ANGLE OF ATTACK
C
C      USER MUST STORE THE NUMBER OF X VALUES IN IZTERM
C      USE STOP 13 FOR ERROR STOPS IN SHOCKG
C
C      DIMENSION ZDUM(1000),RSDUM(1000),RCDUM(1000),SIDUM(1000),
1 CODUM(1000),XC(1000)
C
C      NEQ A 12-16-68
C      Z/L=COSH(R/L)-1.0
C      L=2.109211 CM
C      NEQ2 INPUT
C
C      EL=2.109216
C      X=0.
C      DRS=.0078125
C      NRS=0
10 NRS=NRS+1
IF(NRS.EQ.1) RSDUM(1)=0.
IF(NRS.NE.1) RSDUM(NRS)=RSDUM(NRS-1)+DRS
ZDUM(NRS)=COSH(RSDUM(NRS))-1.0
XC(NRS)=SQRT(2.*ZDUM(NRS)+ZDUM(NRS)**2)
CODUM(NRS)=XC(NRS)/SQRT(XC(NRS)**2+1.0)
RCDUM(NRS)=1.0+XC(NRS)**2

```

APPENDIX A - Continued

```

SIDUM(NRS)= SQRT(1.0-CODUM(NRS)**2)
RCDUM(NRS)=EL*RCDUM(NRS)
XC (NRS)=EL*XC (NRS)
RSDUM(NRS)=EL*RSDUM(NRS)
Z DUM(NRS)=EL*Z DUM(NRS)
IF(ZDUM(NRS).LT.ZSTERM) GO TO 10
X=0.
NOX=0
PRINT 25
25  FORMAT (5X,1HX,16X,2HZS,15X,2HRS,15X,2HRC,15X,4HCOST,13X,4HSINT/)
30  NOX=NOX+1
    IF (NOX.LT.7) X=X+DELX/5.
    IF (NOX.EQ.1) X=0.
    IF (NOX.GT.6) X=X+DELX
    CALL FTLUP (X,ZS,1,NRS,XC,ZDUM)
    CALL FTLUP (X,RS,1,NRS,XC,RSDUM)
    CALL FTLUP (X,RC,1,NRS,XC,RCDUM)
    CALL FTLUP (X,COST,1,NRS,XC,CODUM)
    CALL FTLUP (X,SINT,1,NRS,XC,SIDUM)
    PRINT 35, X,ZS,RS,RC,COST,SINT,NOX
35  FORMAT (6E17.8,15)
    CALL RECOU (10,1,0,X,ZS,RS,RC,COST,SINT)
    IF (ZS.LT.0.0) PRINT 45
45  FORMAT(16H ZS IS NEGATIVE )
    IF(ZS.LT.0.0) STOP 13
C                                     STOP 13          STOP 13
    IF (ZS.LT.ZSTERM) GO TO 30
    IZTERM=NOX
    END FILE 10
    REWIND 10
    RETURN
    END

    SUBROUTINE CALINTH(VAR,DER,ELE1,ELE2,CI,SPEC,N,CUVAR,ELT,
1C1MAX,NERR,PHMAX)
C  ----- IN THE CALINTH VERSION OF CALINT THE VARIABLE IN VAR(2) AND
C  ----- CUVAR(2) MAY BE + OR -.VALUES OF OTHER DEPENDENT VARIABLES
C  ----- ARE EXPECTED TO BE PLUS.                                10-69
    DOUBLE PRECISION VAR
    DIMENSION VAR(52),DER(51),ELE1(51),ELE2(51),CUVAR(52),F1(51),
1F2(51),F3(51),CAPF1(51),CAPF2(51),CAPF3(51),P(51),PH(51),
2DELTY(51),Y3(51),Y4(51),F4(51),Y2(51)
C
C  NERR=1          CI OR N IS EQUAL TO ZERO
C
C  NERR=2          ELE1 LESS THAN OR EQUAL TO ELE2
C
C  TEST INPUT
C
    FN=N
    TEST=CI*FN
    IF(TEST)998,997,999
997 NERR=1
    RETURN
998 IF(ELE1-ELE2)999,999,1000
999 NERR=2
    RETURN
1000 IF(SPEC)5,1,5
C
C  SECTION FOR INITIALIZATION COMPUTATION OF DERIVATIVES
C
    1 SPEC=CI
    ICONT=1
    2 N1=N+1
    DO 3 I=1,N1

```

APPENDIX A - Continued

```

C
3 CUVAR(I)=VAR(I)
  CALL BASIC
C
C      RETURN WITH DERIVATIVES IN DER
C
  DO 4 I=1,N
4 F1(I)=DER(I)
C
  RETURN
C
  COMPUTE Y2,X2
C
5 CUVAR(I)=VAR(I)+CI/2.
  DO 6 I=1,N
    I1=I+1
    Y2(I)=VAR(I1)+CI/2.*F1(I)
    IF(I.EQ.1) GO TO 6
    IF(Y2(I))65,6,6
6 CUVAR(I1)=Y2(I)
  GO TO 66
65 SPEC=CI
  CI=CI/2.
  GO TO 5
C
  CALL BASIC TO EVALUATE F2
C
66 CALL BASIC
C
  RETURN
C
  DO 7 I=1,N
    I1=I+1
    F2(I)=DER(I)
C
  COMPUTE Y3
C
Y3(I)=VAR(I1)+CI/2.*F2(I)
  IF(I.EQ.1) GO TO 7
  IF(Y3(I))65,7,7
7 CUVAR(I1)=Y3(I)
C
  CALL BASIC TO EVALUATE F3
C
  CALL BASIC
  RETURN
C
  DO 10 I=1,N
    F3(I)=DER(I)
C
  COMPUTE P,PH AND CAP F TERMS
C
  IF(Y3(I)-Y2(I)) 9,8,9
8 P(I)=0.
  GO TO 91
9 P(I)=-((F3(I)-F2(I))/(Y3(I)-Y2(I)))
91 PH(I)=P(I)*CI
  IF(PH(I))83,83,103
83 PH(I)=0.
  P(I)=0.
  GO TO 84
103 IF(ABS(Y3(I)-Y2(I))/((ABS(Y3(I))+ABS(Y2(I)))/2.)-.5E-4)83,83,84
84 IF(PH(I)-.1)85,85,95
85 CAPF1(I)=1.-PH(I)/2.+(PH(I)**2)/6.-(PH(I)**3)/24.

```

APPENDIX A - Continued

```

CAPF2(I)=.5-PH(I)/6.+(PH(I)**2)/24.-(PH(I)**3)/120.
CAPF3(I)=1./6.-PH(I)/24.+(PH(I)**2)/120.-(PH(I)**3)/720.
GO TO 10
95 CAPF1(I)=(EXP(-PH(I))-1.)/(-PH(I))
CAPF2(I)=(CAPF1(I)-1.)/(-PH(I))
CAPF3(I)=(CAPF2(I)-.5)/(-PH(I))
10 CONTINUE

C
C      IS PH BETWEEN ELE2 AND ELE1
C
      IF(ICONT-1)101,101,102
102 ICONT=ICONT-1
      SPEC=CI
      GO TO 17
101 DO 11 I=1,N
104 IF(ABS(PH(I))-ELE1(I))11,11,13
      11 CONTINUE

C
      12 SPEC=CI
      GO TO 15

C
C      HALVE INTERVAL AND DOUBLE PH RANGE
C
      13 DO 96 I=1,N
          ELE1(I)=ELE1(I)*2.
          IF(ELE1(I)-PHMAX)94,94,955
          94 ELE2(I)=ELE2(I)*2.
          GO TO 96
          955 ELE1(I)=ELE1(I)/2.
          96 CONTINUE
          SPEC=CI

          CI=CI/2.
          ICONT=3
          GO TO 5

C
C      RETURN TO RECOMPUTE INTERVAL
C
C
C      RETURN TO RECOMPUTE INTERVAL
C
      15 DO 16 I=1,N
          IF(ABS(PH(I))-ELE2(I))16,17,17
          16 CONTINUE

C
C      DOUBLE INTERVAL
C
          CI=2.*CI
          IF(CI-CIMAX)17,17,165
          165 CI=CIMAX
          17 CONTINUE

C
C      COMPUTE Y4,X4
C
          DO 18 I=1,N
              I1=I+1
              CUVAR(I1)=VAR(I1)+SPEC*(F3(I)*(2.*CAPF2(I))+F1(I)*
              1(CAPF1(I)-2.*CAPF2(I))+F2(I)*PH(I)*CAPF2(I))
              IF(I.EQ.1) GO TO 18
              IF(CUVAR(I1))175,18,18
          175 CI=SPEC
              CI=CI/2.
              GO TO 5
          18 Y4(I)=CUVAR(I1)

C
          CUVAR(1)=VAR(1)+SPEC

```

APPENDIX A - Continued

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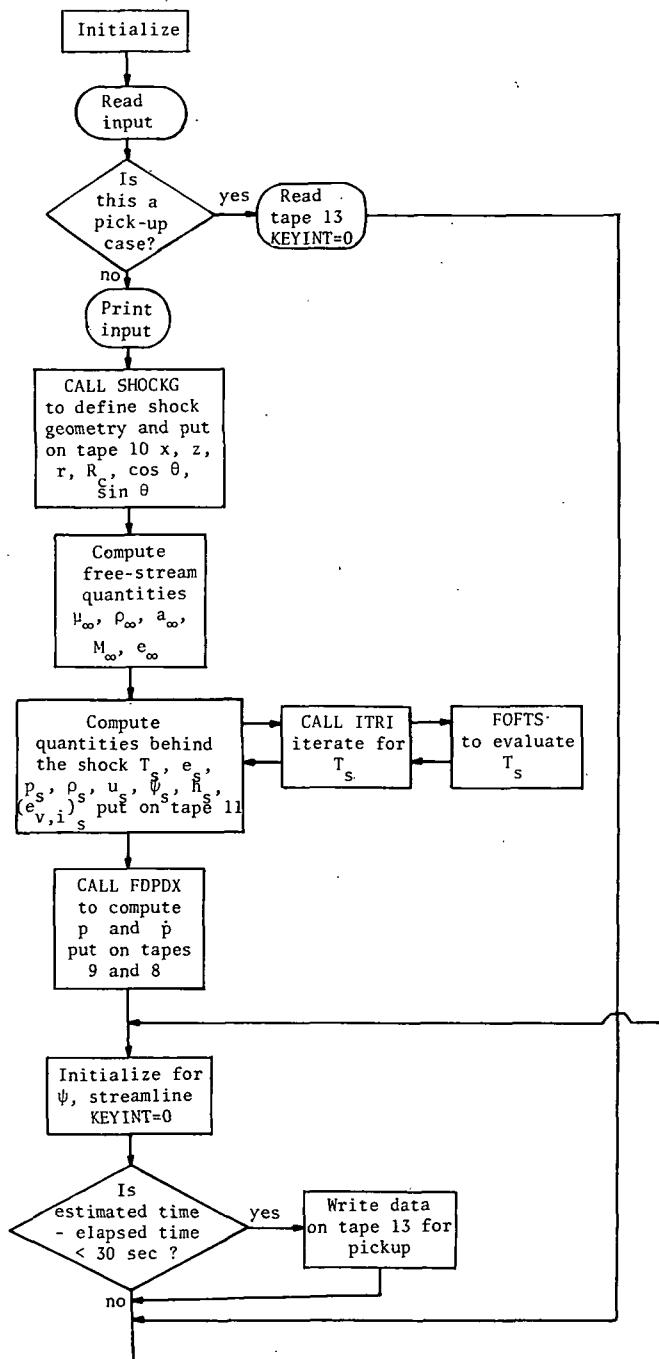
C
C      CALL BASIC TO EVALUATE F4
C
C      CALL BASIC
C      RETURN
C
C      DO 20 I=1,N
C      I1=I+1
C      F4(I)=DER(I)
C
C      COMPUTE DELTA Y
C
C      DELTY(I)=SPEC*(F1(I)*CAPF1(I)+(-3.*(F1(I)+P(I)*VAR(I1))
C      1+2.*(F2(I)+P(I)*Y2(I))+2.*(F3(I)+P(I)*Y3(I))-F4(I)
C      2-P(I)*Y4(I))*CAPF2(I)+4.*((F1(I)+P(I)*VAR(I1))-(F2(I)
C      3+P(I)*Y2(I))-(F3(I)+P(I)*Y3(I))+(F4(I)+P(I)*Y4(I)))*
C      4CAPF3(I))
C
C      COMPUTE Y+DELTA Y
C
C      20 CUVAR(I1)=VAR(I1)+DELTY(I)
C
C      CALL CHECK FOR DECISION TO ACCEPT OR RECCMPUTE
C      INTERVAL
C      CALL CHECK
C      IF (ELT)21,21,23
C
C      UPDATE Y VALUES
C
C      21 N1=N+1
C      DO 22 I=2,N1
C      I1=I-1
C      22 VAR(I)=VAR(I)+DELTY(I1)
C      VAR(I)=VAR(I)+SPEC
C
C      RETURN TO COMPUTE DERIVATIVES AT Y+DELTA Y
C
C      GO TO 2
C
C      RETURN TO RECCMPUTE INTERVAL
C
C      23 GO TO 5
C
C      END

```

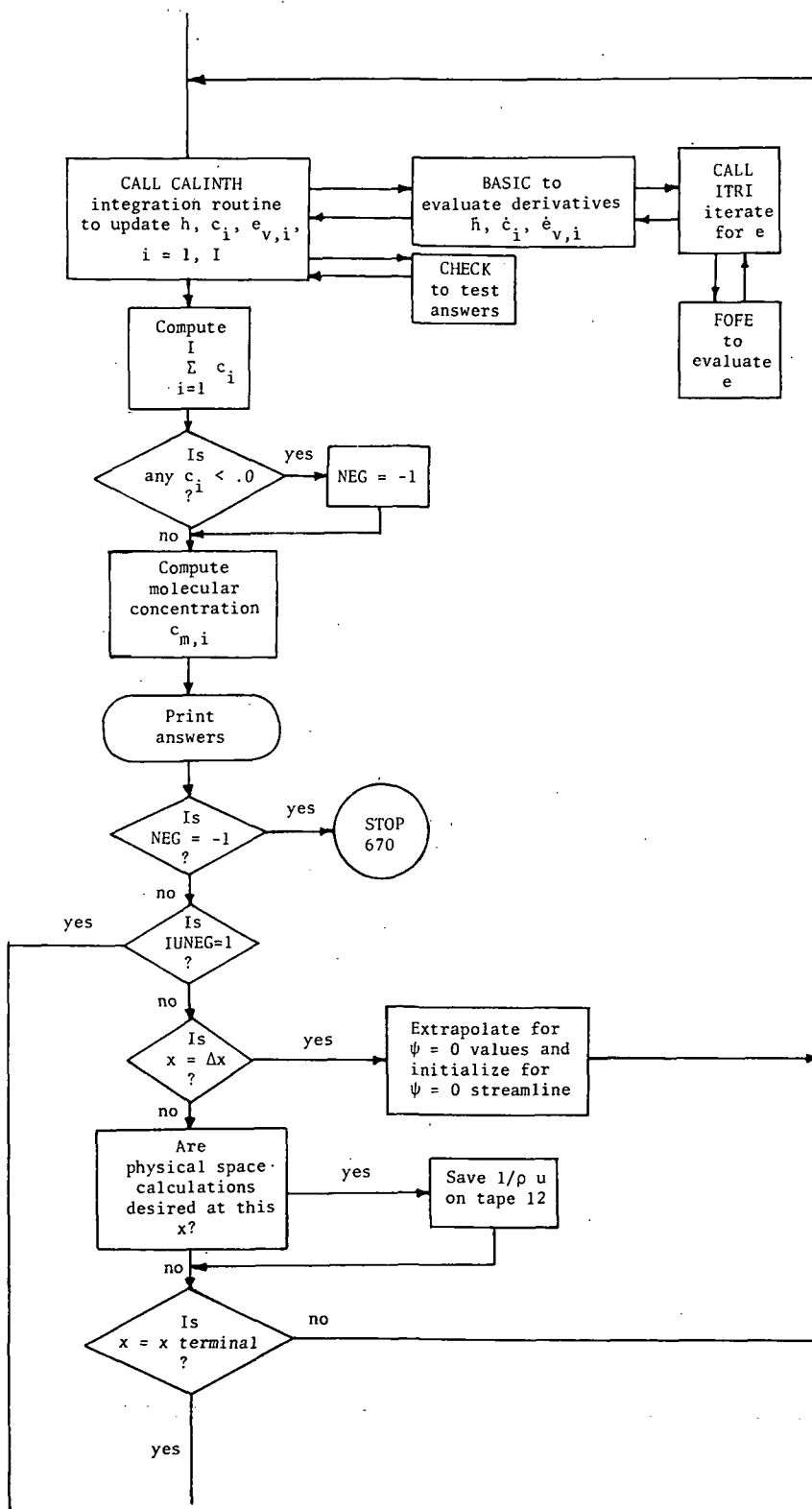
APPENDIX A - Continued

The flow charts for the program are presented below:

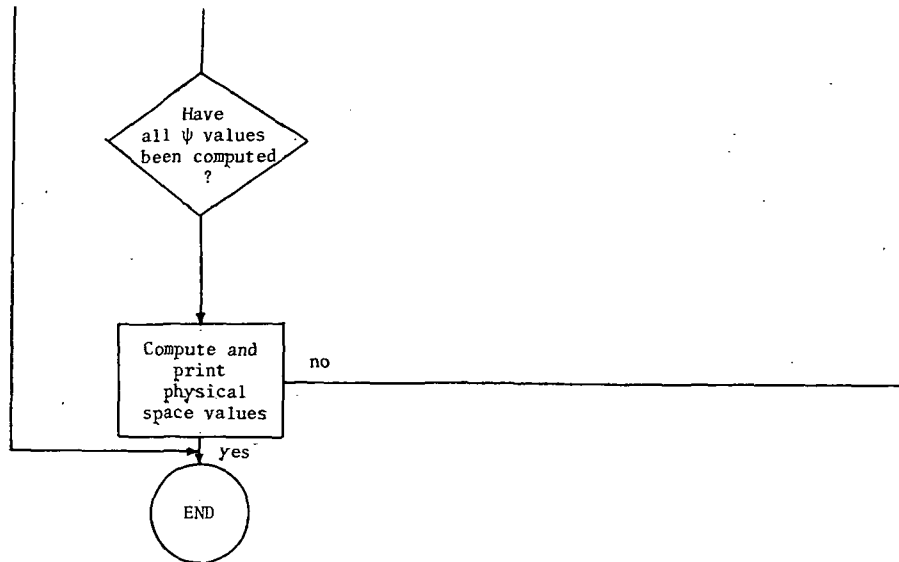
D1290



APPENDIX A - Continued



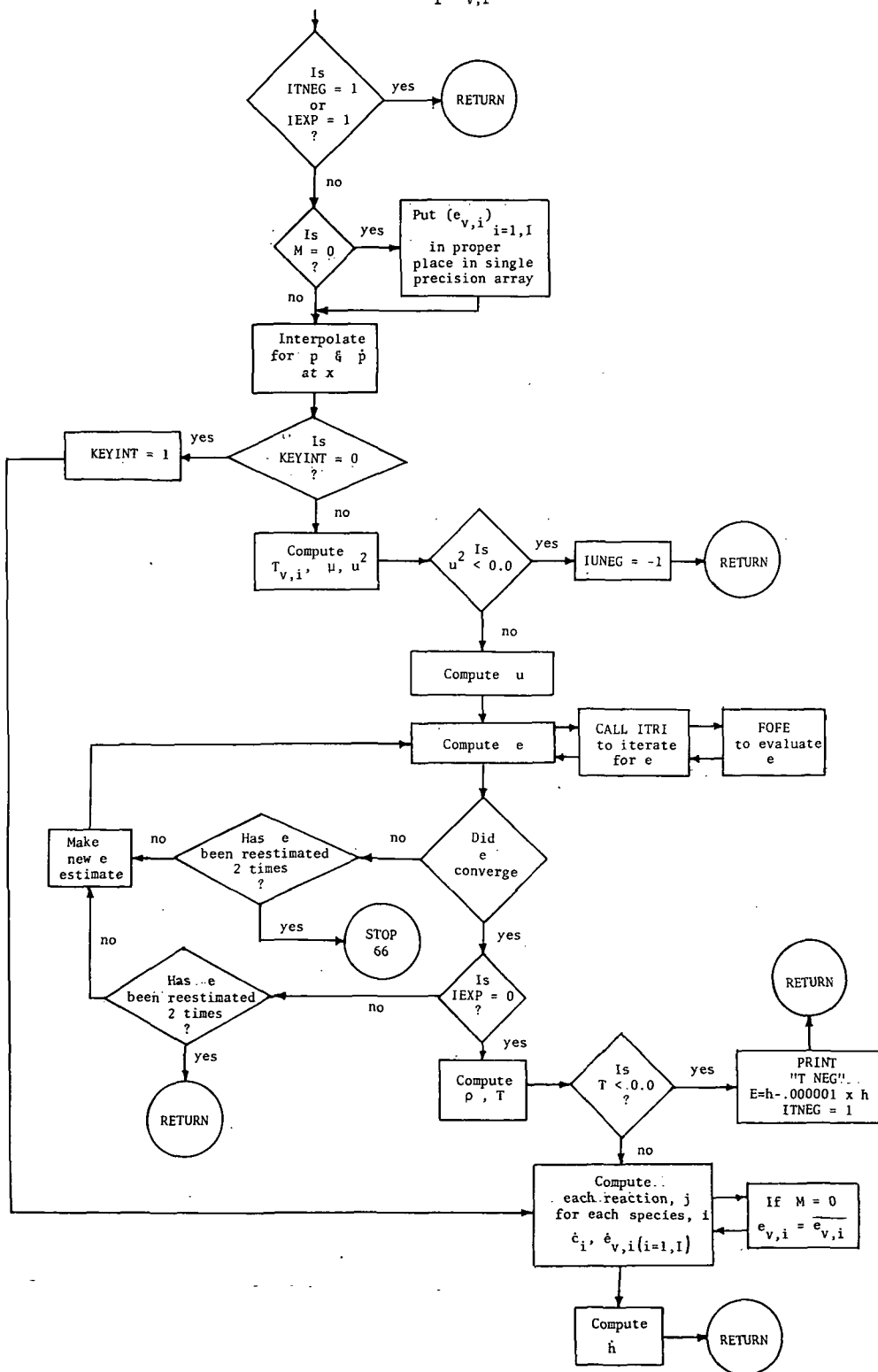
APPENDIX A -- Continued



APPENDIX A - Continued

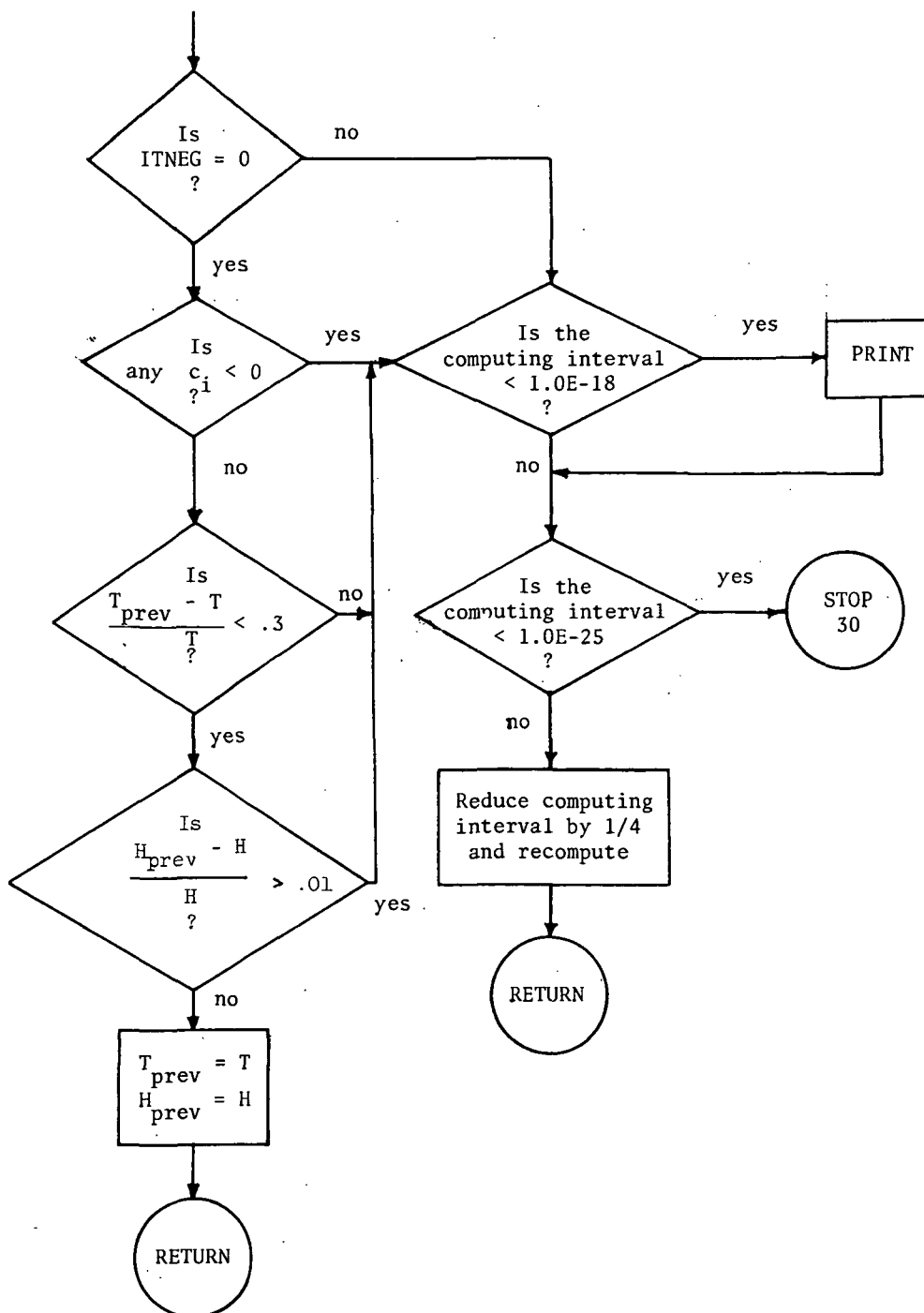
BASIC

Evaluate derivatives $\dot{c}_i, \dot{e}_{v,i}, h$ $i = 1, I$



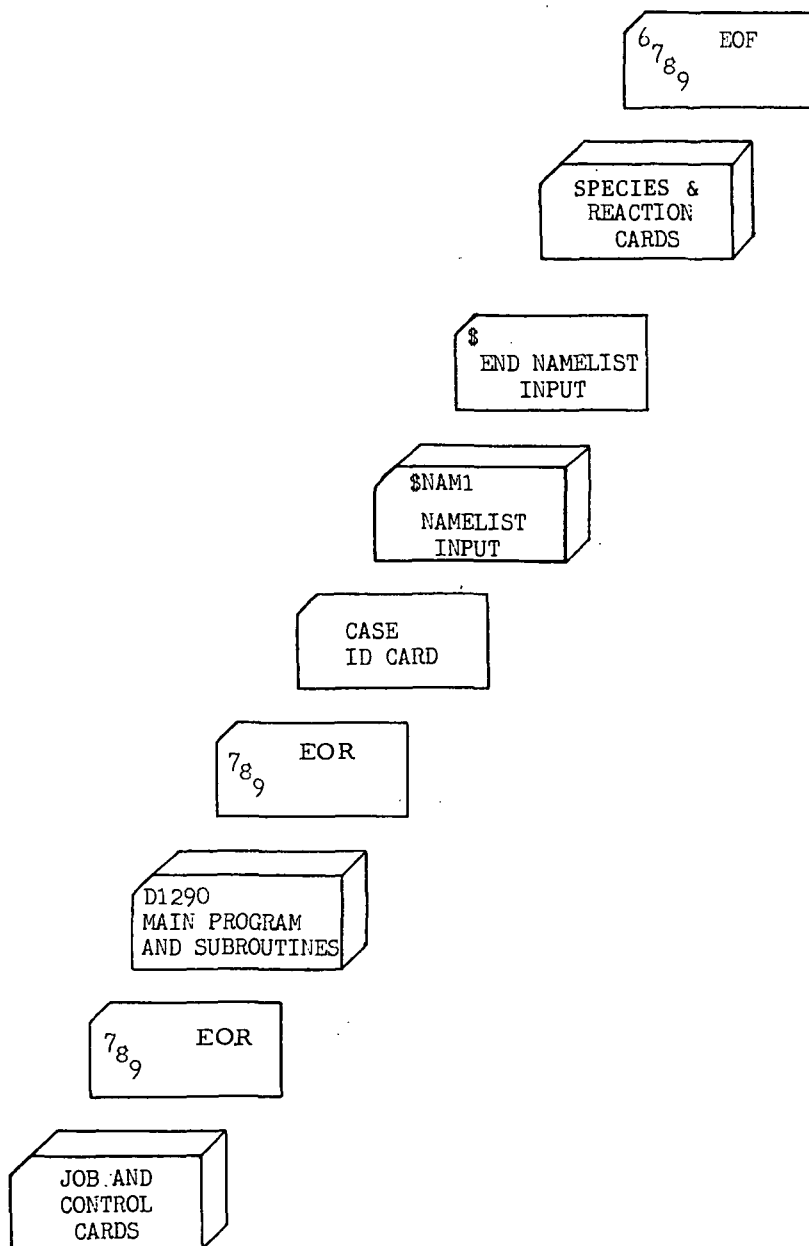
CHECK

Test answers



APPENDIX A - Concluded

The deck setup is as follows:



APPENDIX B

GENERAL RATE EQUATION

In the case of a rate expression being the same for several catalytic species, it is desirable for the sake of convenience to incorporate all these catalysts into one reaction. In order to incorporate these catalysts, the set of catalytic species is treated as a general species designated as M . Those species denoted by M will be related to the j th reaction by a set of input parameters $a_{i,j}$. Thus, if the i th species is one of the set composing M in the j th reaction, $a_{i,j}$ will be unity; otherwise, $a_{i,j}$ will be zero.

If a general species M is included in the general rate expression of equation (34),

$$\left[\left(\frac{\partial c_i}{\partial x} \right) \psi \right]_j = \left[\frac{K_j \mu_i}{\rho u} (\nu'_{i,j} - \nu_{i,j}) \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i} \right)^{\nu_{i,j}} \right] \left(\frac{\rho c_M}{\mu_M} \right)^{\nu_{I+1,j}} \quad (B1)$$

where the general species is denoted by the subscript $I + 1$. The mass fraction of M , that is, c_M is

$$c_M = \sum_{i=1}^I a_{i,j} c_i \quad (B2)$$

and the molecular weight μ_M is

$$\mu_M = \sum_{i=1}^I m_i \mu_i \quad (B3)$$

m_i being the mole fraction of the i th component of the set composing M . Hence,

$$m_i = \frac{p_{M,i}}{p_M} \quad (B4)$$

and

$$p_{M,i} = \frac{c_i \mu}{\mu_i} p a_{i,j} \quad (B5)$$

By using Dalton's law of partial pressures

$$p_M = \sum_{i=1}^I p_{M,i} \quad (B6)$$

APPENDIX B - Concluded

Substituting the three relations (eqs. (A4), (A5), and (A6)) into equation (A3) results in

$$\mu_M = \frac{\sum_{i=1}^I c_i a_{i,j}}{\sum_{i=1}^I \frac{c_i a_{i,j}}{\mu_i}} \quad (B7)$$

Inclusion of equations (A2) and (A7) into equation (A1) yields a rate equation incorporating the general species M,

$$\left[\left(\frac{\partial c_i}{\partial x} \right)_{\psi} \right]_j = \left[\frac{K_j \mu_i}{\rho u} (\nu'_{i,j} - \nu_{i,j}) \prod_{i=1}^I \left(\frac{\rho c_i}{\mu_i} \right)^{\nu_{i,j}} \right] \left(\rho \sum_{i=1}^I \frac{c_i a_{i,j}}{\mu_i} \right)^{\nu_{I+1,j}} \quad (B8)$$

APPENDIX C

SPECIES, REACTIONS, AND RATES FOR CASES I TO V

The species, reactions, and rates for Cases I to V are presented in this appendix.

Cases I and II

The species are N_2 , N , O_2 , O , NO , NO^+ , and e^- for Cases I and II.

Number	Reaction	Rates	Reference
1	$O_2 + M \rightarrow 2O + M$	$1.2 \times 10^{21} T^{-3/2} \exp\left(-\frac{59\,380}{T}\right)$	8
2	$2O + M \rightarrow O_2 + M$	$1.0 \times 10^{18} T^{-1}$	8
3	$NO + M \rightarrow N + O + M$	$5.2 \times 10^{21} T^{-3/2} \exp\left(-\frac{75\,490}{T}\right)$	8
4	$N + O + M \rightarrow NO + M$	$1.3 \times 10^{21} T^{-3/2}$	8
5	$N_2 + M \rightarrow 2N + M$	$3.0 \times 10^{21} T^{-3/2} \exp\left(-\frac{113\,260}{T}\right)$	8
6	$2N + M \rightarrow N_2 + M$	$1.67 \times 10^{20} T^{-3/2}$	8
7	$N + O_2 \rightarrow NO + O$	$1.0 \times 10^{12} T^{1/2} \exp\left(-\frac{3120}{T}\right)$	8
8	$NO + O \rightarrow N + O_2$	$2.38 \times 10^{11} T^{1/2} \exp\left(-\frac{19\,130}{T}\right)$	8
9	$N_2 + O \rightarrow NO + N$	$5.0 \times 10^{13} \exp\left(-\frac{38\,000}{T}\right)$	8
10	$NO + N \rightarrow N_2 + O$	1.11×10^{13}	8
11	$N_2 + O_2 \rightarrow 2NO$	$9.1 \times 10^{24} T^{-5/2} \exp\left(-\frac{65\,000}{T}\right)$	8
12	$2NO \rightarrow N_2 + O_2$	$4.79 \times 10^{23} T^{-5/2} \exp\left(-\frac{43\,270}{T}\right)$	8
13	$NO^+ + e^- \rightarrow N + O$	$1.8 \times 10^{21} T^{-3/2}$	8
14	$N + O \rightarrow NO^+ + e^-$	$2.17 \times 10^{11} T^{0.12} \exp\left(-\frac{31\,858}{T}\right)$	8

APPENDIX C - Continued

Case III

The species are CO_2 , CO , CO^+ , C_2 , C , O , C^+ , O^+ , and e^- for Case III.

Number	Reaction	Rates	Reference
1	$\text{CO}_2 + \text{M} \rightarrow \text{CO} + \text{O} + \text{M}$	$6.955 \times 10^{12} T^{1/2} \exp\left(-\frac{63\,286}{T}\right)$	36
2	$\text{CO} + \text{O} + \text{M} \rightarrow \text{CO}_2 + \text{M}$	$3.39 \times 10^6 T^{1.6175}$	36
3	$\text{CO} + \text{M} \rightarrow \text{C} + \text{O} + \text{M}$	$7.72 \times 10^{12} T^{1/2} \exp\left(-\frac{128\,925}{T}\right)$	36
4	$\text{C} + \text{O} + \text{M} \rightarrow \text{CO} + \text{M}$	$2.26 \times 10^8 T^{0.7366} \exp\left(\frac{665}{T}\right)$	36
5	$\text{C} + \text{O} \rightarrow \text{CO}^+ + e^-$	$2.049 \times 10^{12} \exp\left(-\frac{33\,300}{T}\right)$	40
6	$\text{CO}^+ + e^- \rightarrow \text{C} + \text{O}$	6.023×10^{16}	40
7	$\text{C} + e^- \rightarrow \text{C}^+ + 2e^-$	$2.09 \times 10^{14} T^{0.5} \exp\left(-\frac{130\,713}{T}\right)$	41
8	$\text{C}^+ + 2e^- \rightarrow \text{C} + e^-$	$9.65 \times 10^{21} T^{-0.836}$	41
9	$\text{O} + e^- \rightarrow \text{O}^+ + 2e^-$	$2.14 \times 10^{14} T^{0.5} \exp\left(-\frac{158\,000}{T}\right)$	41
10	$\text{O}^+ + 2e^- \rightarrow \text{O} + e^-$	$6.05 \times 10^{22} T^{-2}$	41
11	$\text{C}_2 + \text{M} \rightarrow 2\text{C} + \text{M}$	$6.74 \times 10^{13} T^{0.5} \exp\left(-\frac{70\,529}{T}\right)$	41
12	$2\text{C} + \text{M} \rightarrow \text{C}_2 + \text{M}$	$1.61 \times 10^{12} T^{0.743}$	41

APPENDIX C - Concluded

Cases IV and V

The species are CO_2 , CO , C , O , A , C^+ , A^+ , and e^- for Cases IV and V.

Number	Reaction	Rates	Reference
1	$\text{CO}_2 + \text{M} \rightarrow \text{CO} + \text{O} + \text{M}$	$6.955 \times 10^{12} T^{1/2} \exp\left(-\frac{63\,286}{T}\right)$	36
2	$\text{CO} + \text{O} + \text{M} \rightarrow \text{CO}_2 + \text{M}$	$3.39 \times 10^6 T^{1.6175}$	36
3	$\text{CO} + \text{M} \rightarrow \text{C} + \text{O} + \text{M}$	$7.72 \times 10^{12} T^{1/2} \exp\left(-\frac{128\,925}{T}\right)$	36
4	$\text{C} + \text{O} + \text{M} \rightarrow \text{CO} + \text{M}$	$2.26 \times 10^8 T^{0.7366} \exp\left(\frac{665}{T}\right)$	36
5	$\text{C} + \text{e}^- \rightarrow \text{C}^+ + 2\text{e}^-$	$2.09 \times 10^{14} T^{0.5} \exp\left(-\frac{130\,713}{T}\right)$	41
6	$\text{C}^+ + 2\text{e}^- \rightarrow \text{C} + \text{e}^-$	$9.65 \times 10^{21} T^{-0.836}$	41
7	$\text{O} + \text{e}^- \rightarrow \text{O}^+ + 2\text{e}^-$	$2.14 \times 10^{14} T^{0.5} \exp\left(-\frac{158\,000}{T}\right)$	41
8	$\text{O}^+ + 2\text{e}^- \rightarrow \text{O} + \text{e}^-$	$6.05 \times 10^{22} T^{-2}$	41
9	$\text{C} + \text{O} \rightarrow \text{CO}^+ + \text{e}^-$	$2.049 \times 10^{12} \exp\left(-\frac{33\,300}{T}\right)$	40
10	$\text{CO}^+ + \text{e}^- \rightarrow \text{C} + \text{O}$	6.023×10^{16}	40
11	$\text{A} + \text{e}^- \rightarrow \text{A}^+ + 2\text{e}^-$	$1.94 \times 10^{14} T^{0.5} \exp\left(-\frac{182\,830}{T}\right)$	41
12	$\text{A}^+ + 2\text{e}^- \rightarrow \text{A} + \text{e}^-$	$8.55 \times 10^{21} T^{-1.075}$	41

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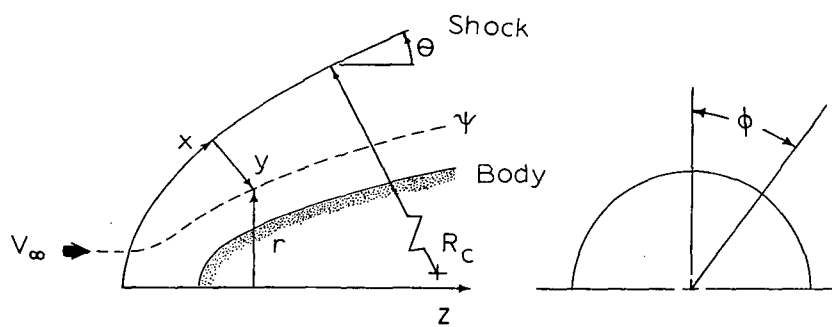


Figure 1.- Shock-oriented coordinate system.

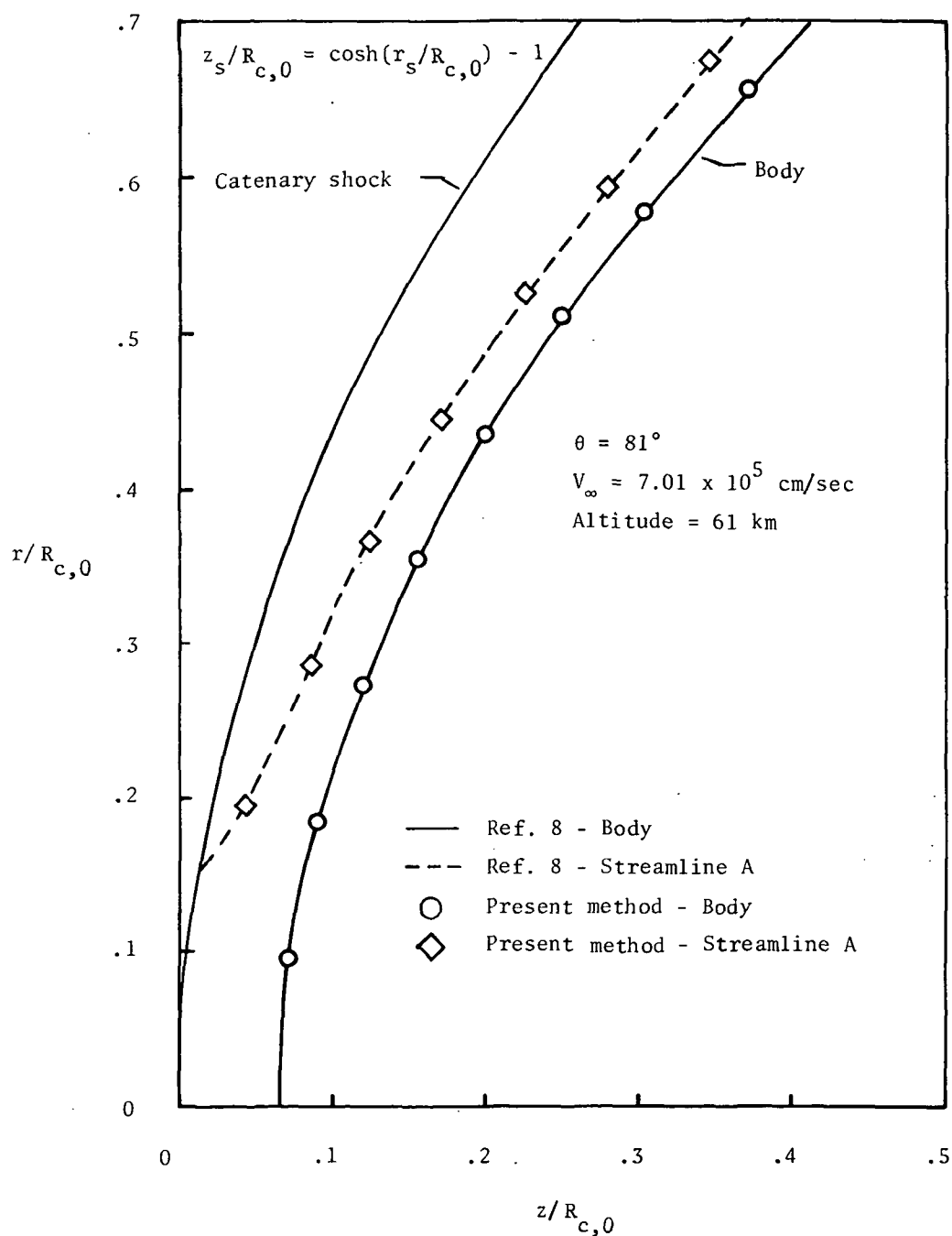


Figure 2.- Comparison of body shape and streamline location crossing the shock at $\theta = 81^\circ$ ($x/R_{c,0} = 0.16$) with exact inverse method for catenary shock. Case I.

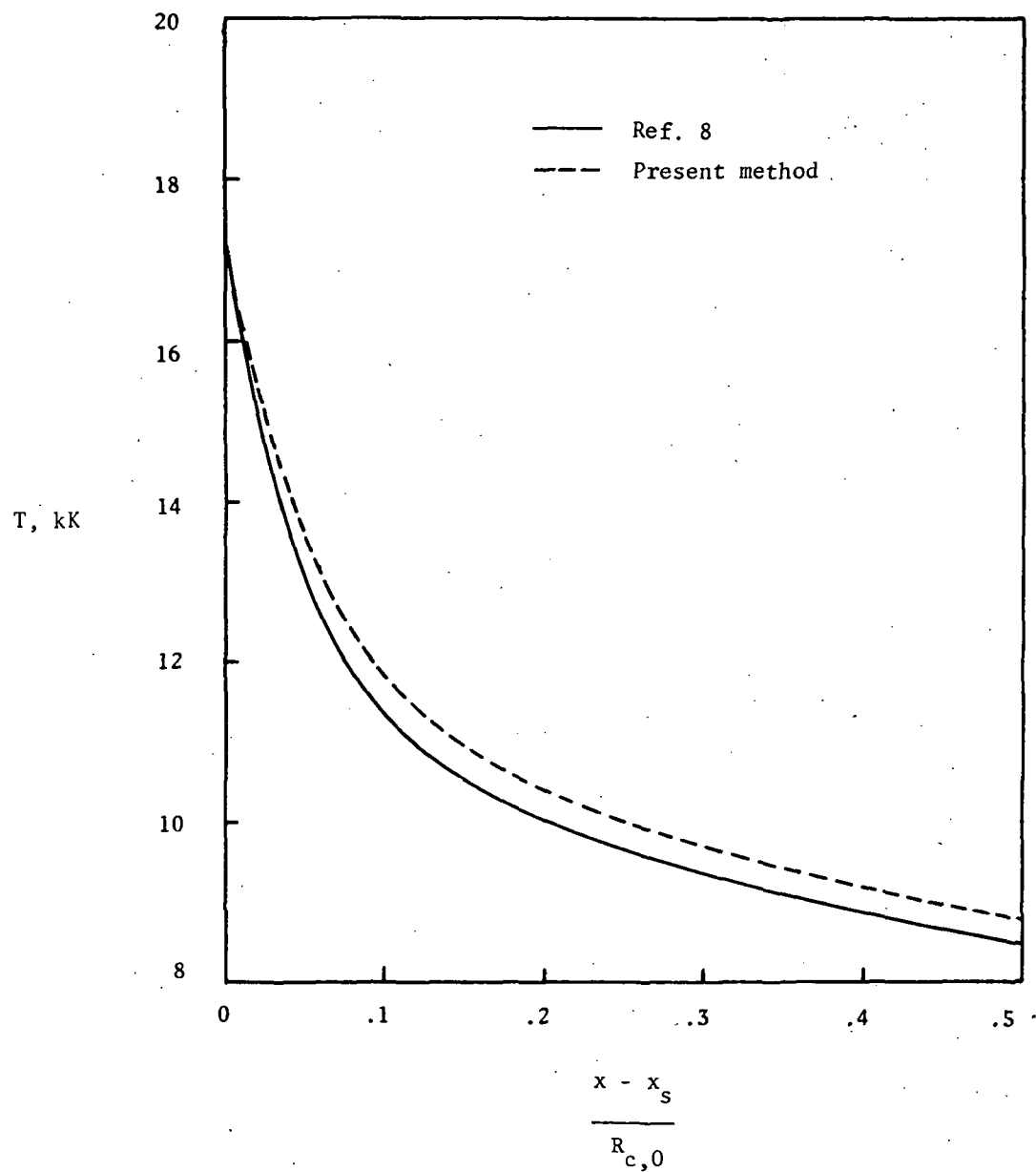


Figure 3.- Temperature variation along streamline A. Case I.

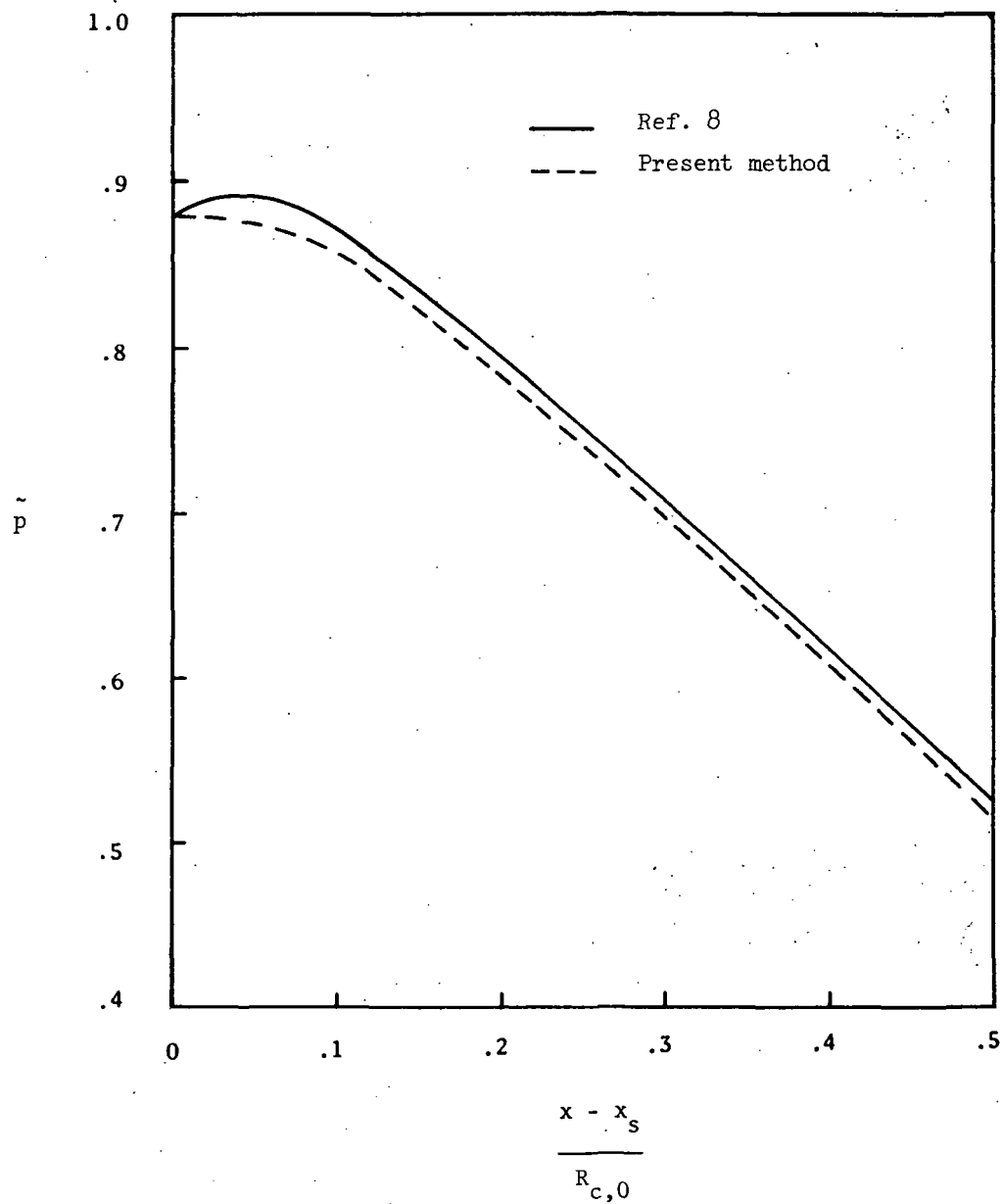


Figure 4.- Pressure variation along streamline A. Case I.

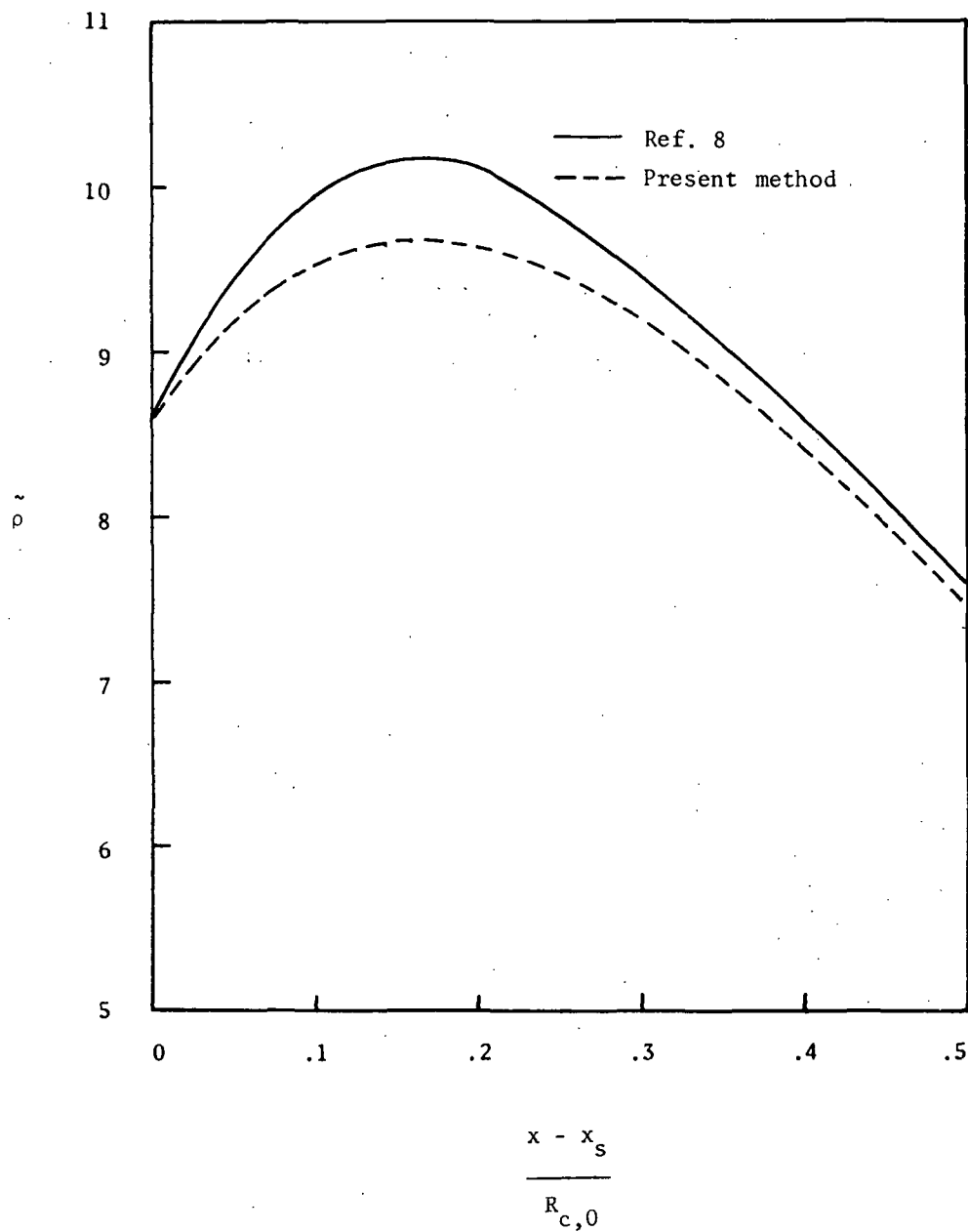
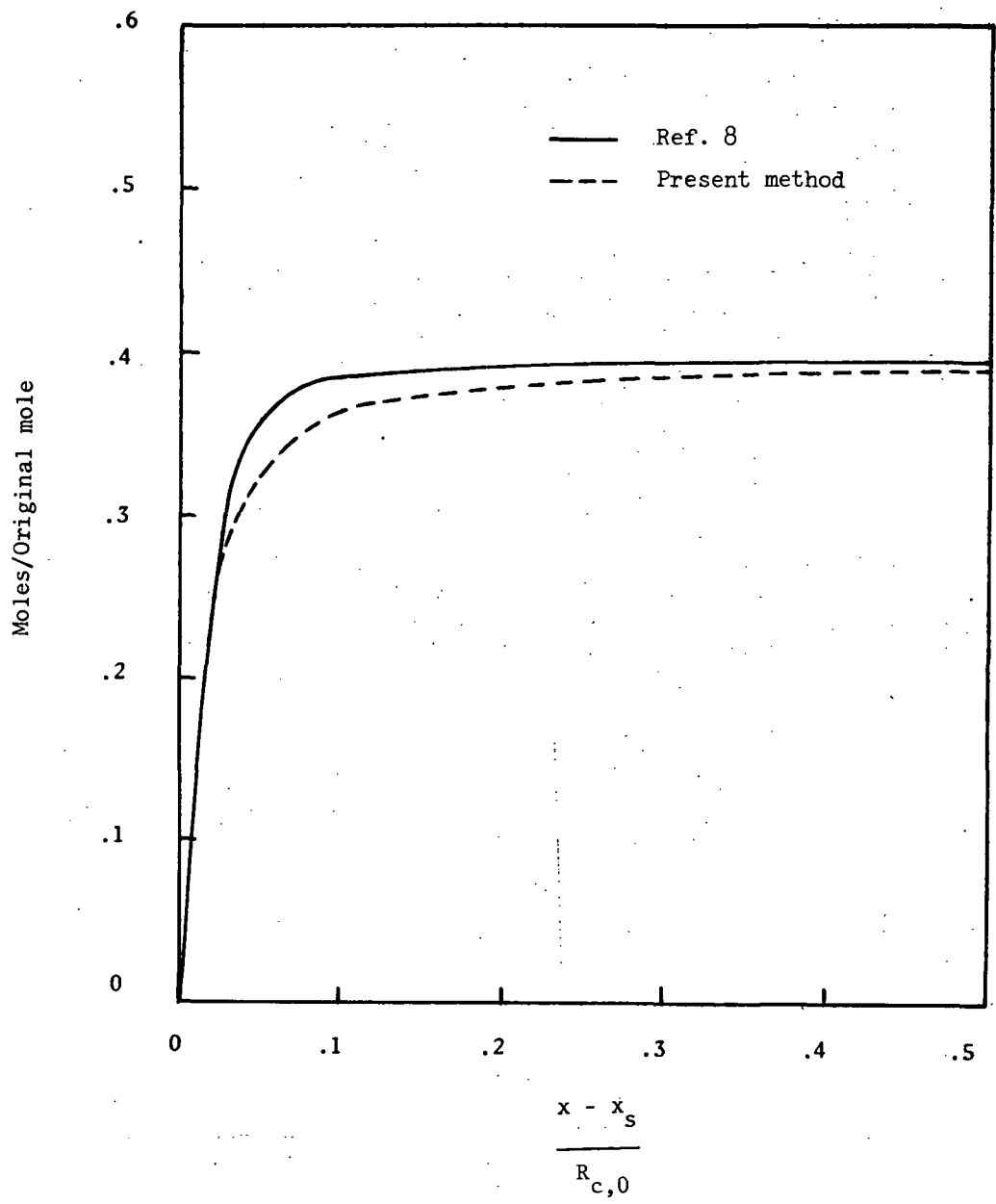
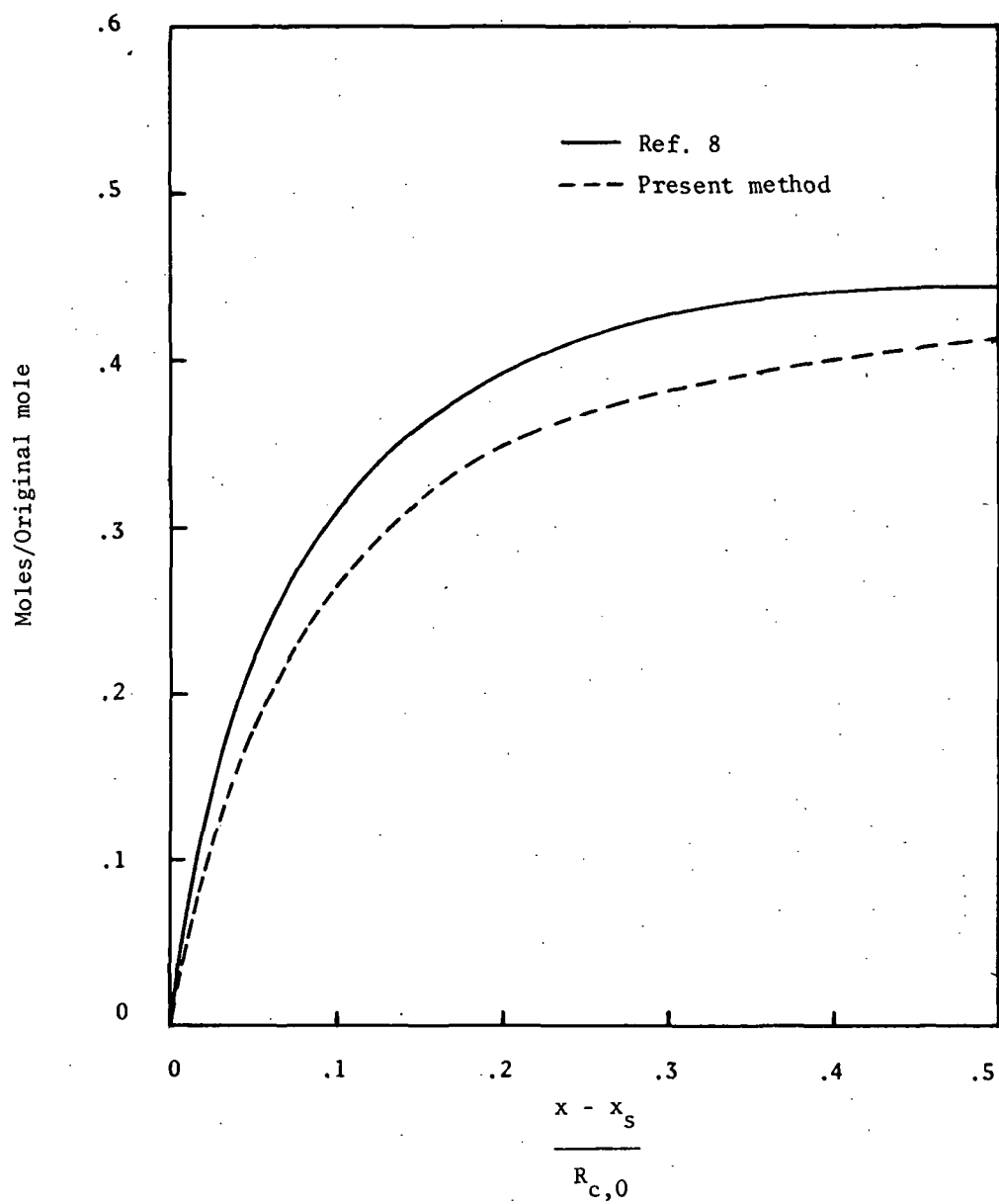


Figure 5.- Density variation along streamline A. Case I.



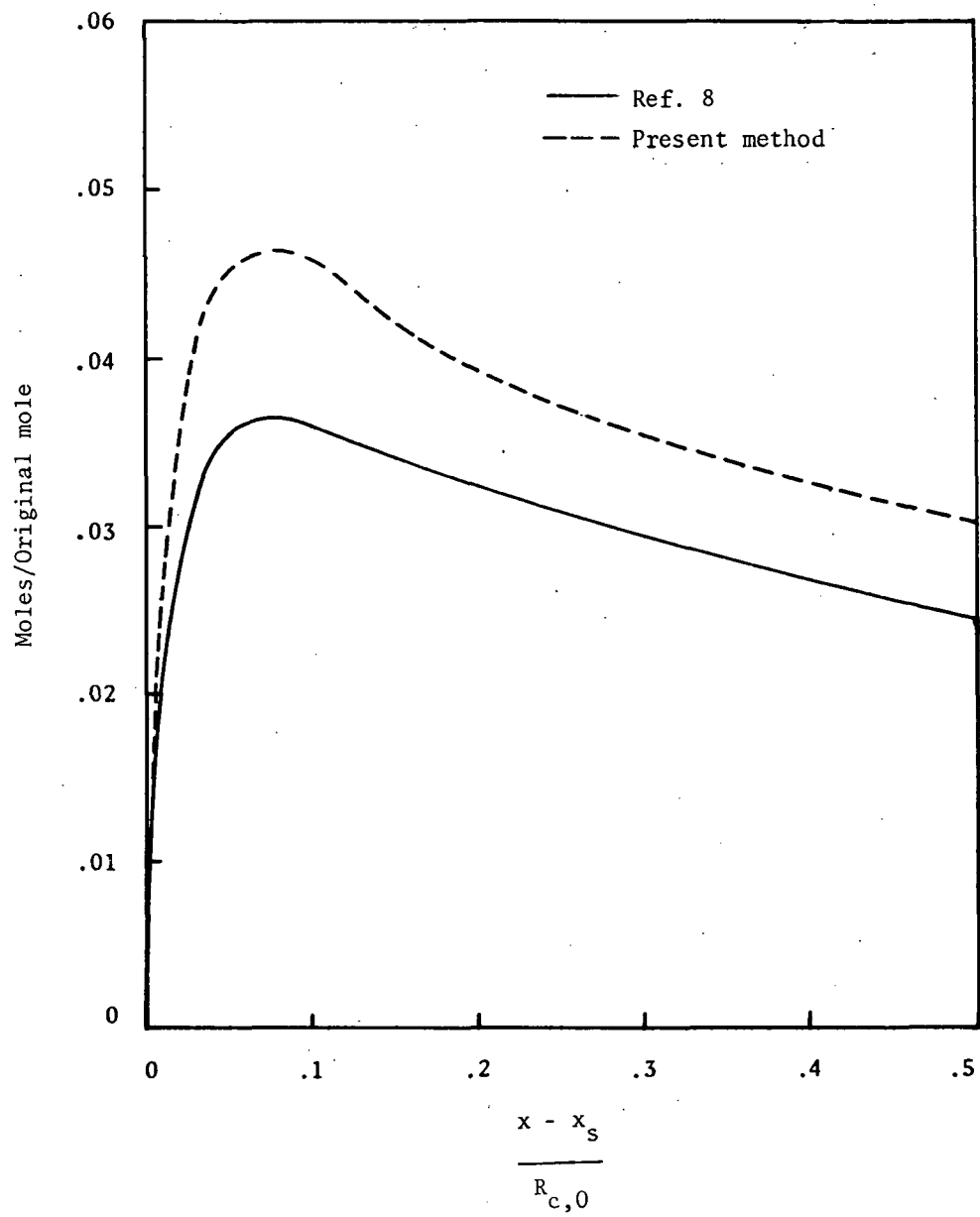
(a) Oxygen atom.

Figure 6.- Concentration variation along streamline A. Case I.



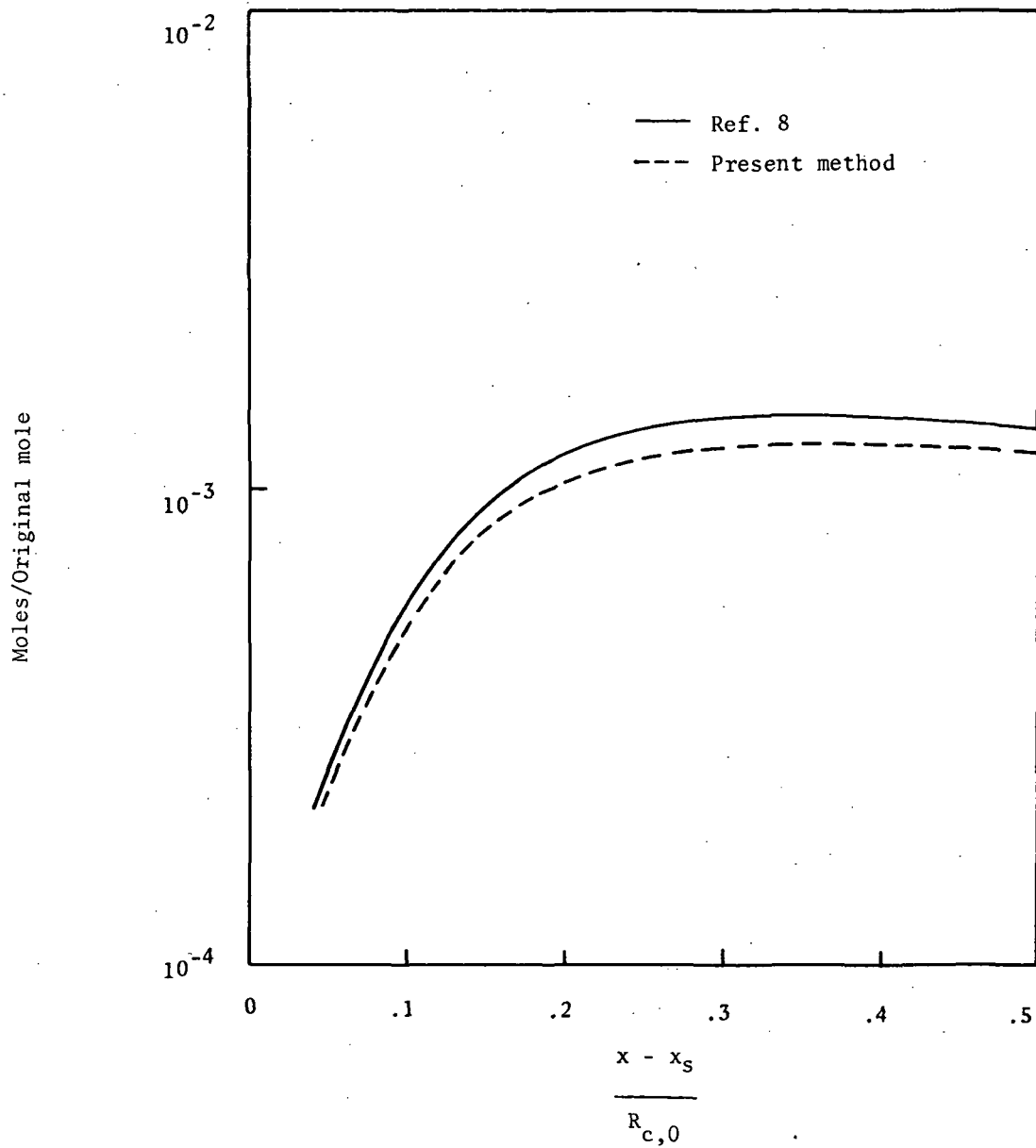
(b) Nitrogen atom.

Figure 6.- Continued.



(c) NO.

Figure 6.- Continued.



(d) Electron.

Figure 6.- Concluded.

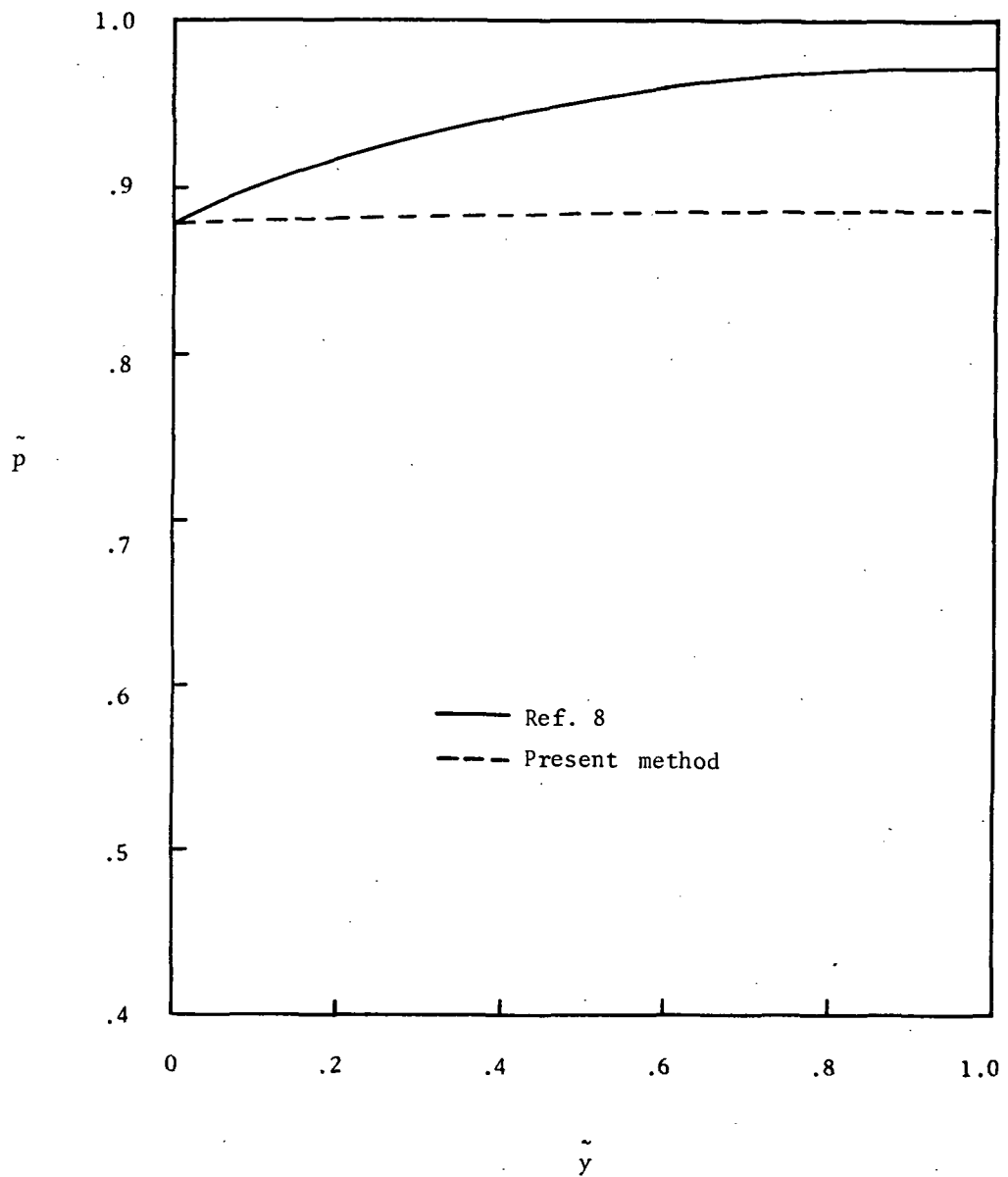


Figure 7.- Pressure variation across shock layer at $\theta = 81^\circ$. Case I.

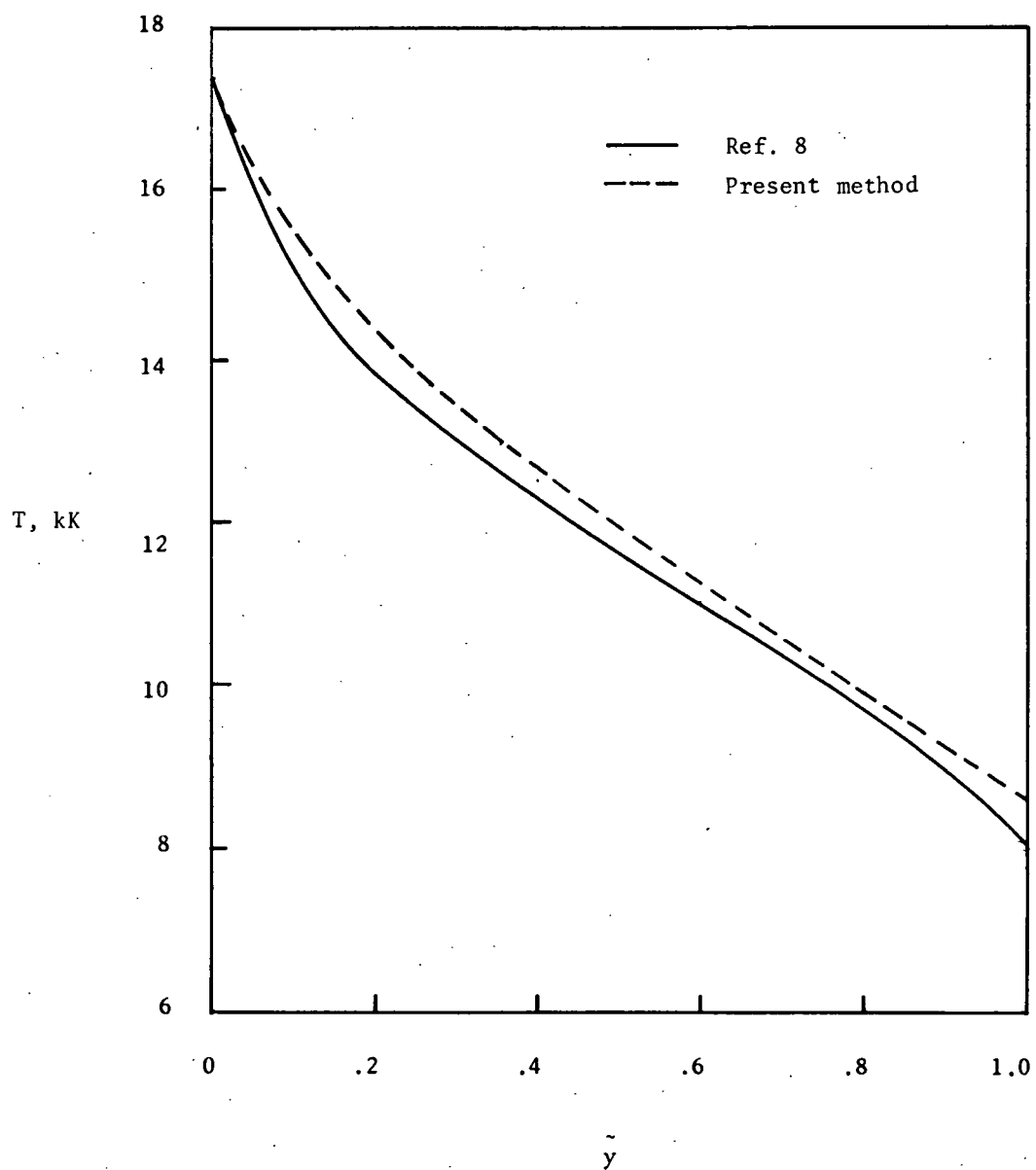


Figure 8.- Temperature variation across shock layer at $\theta = 81^\circ$. Case I.

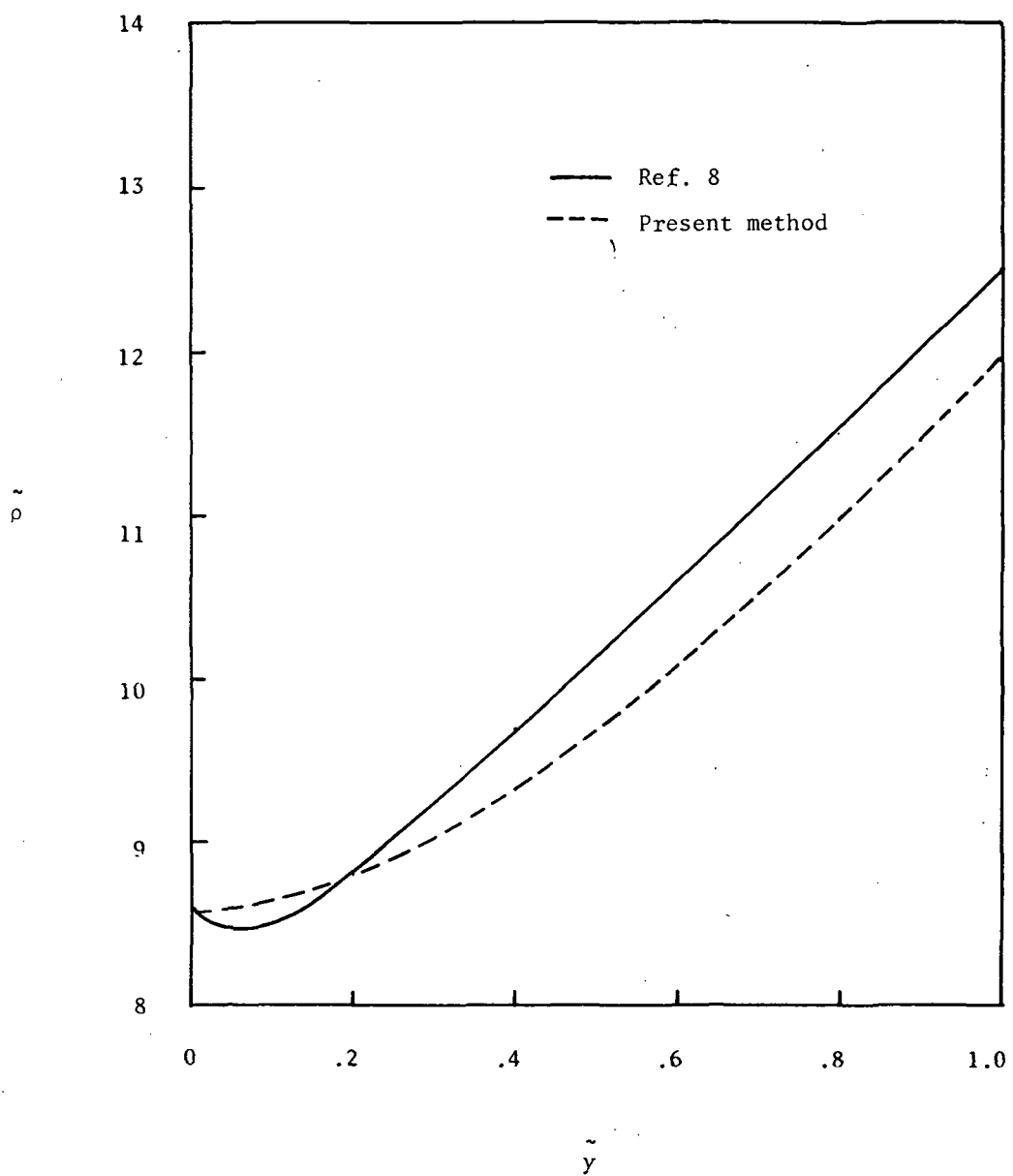
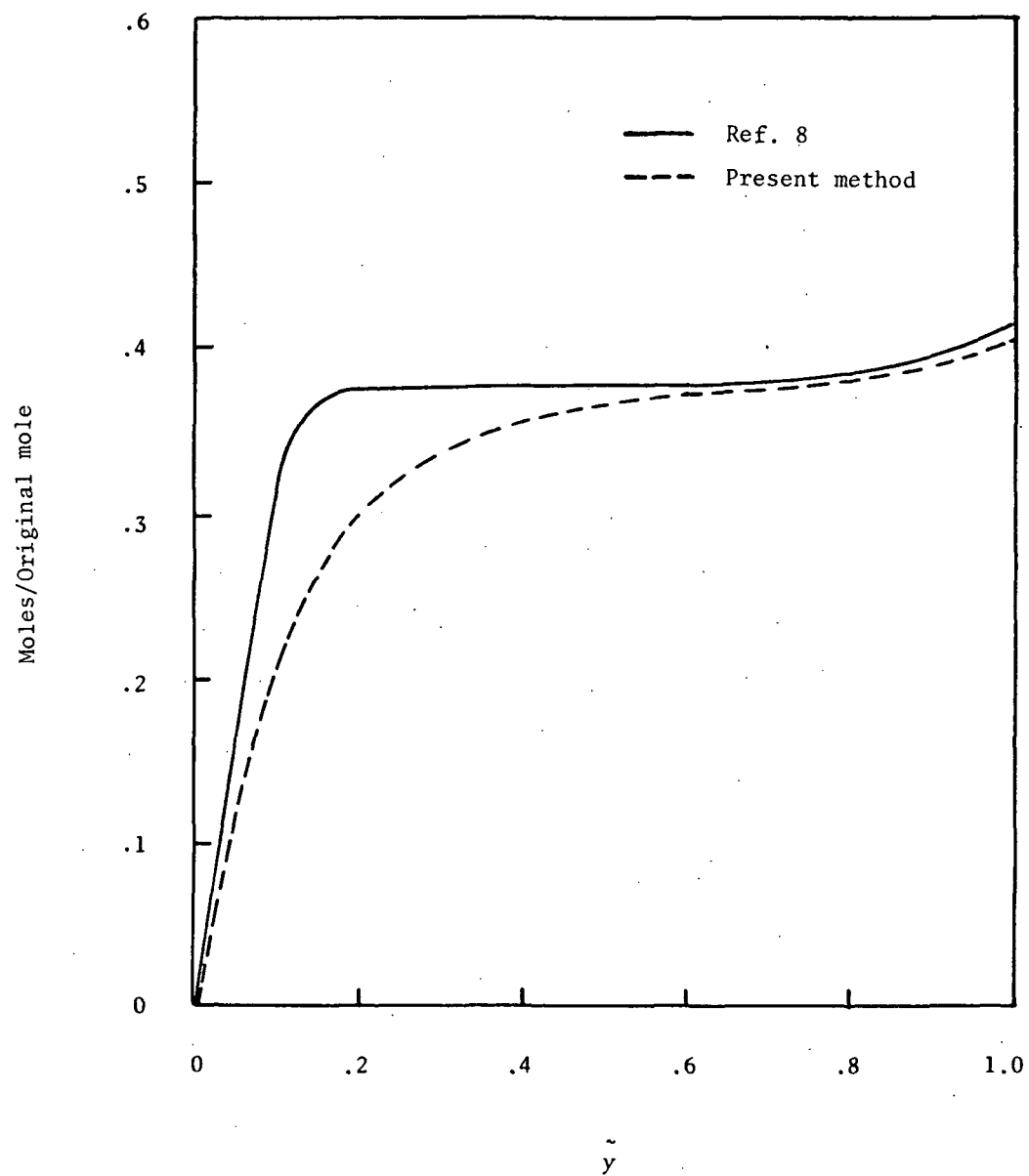
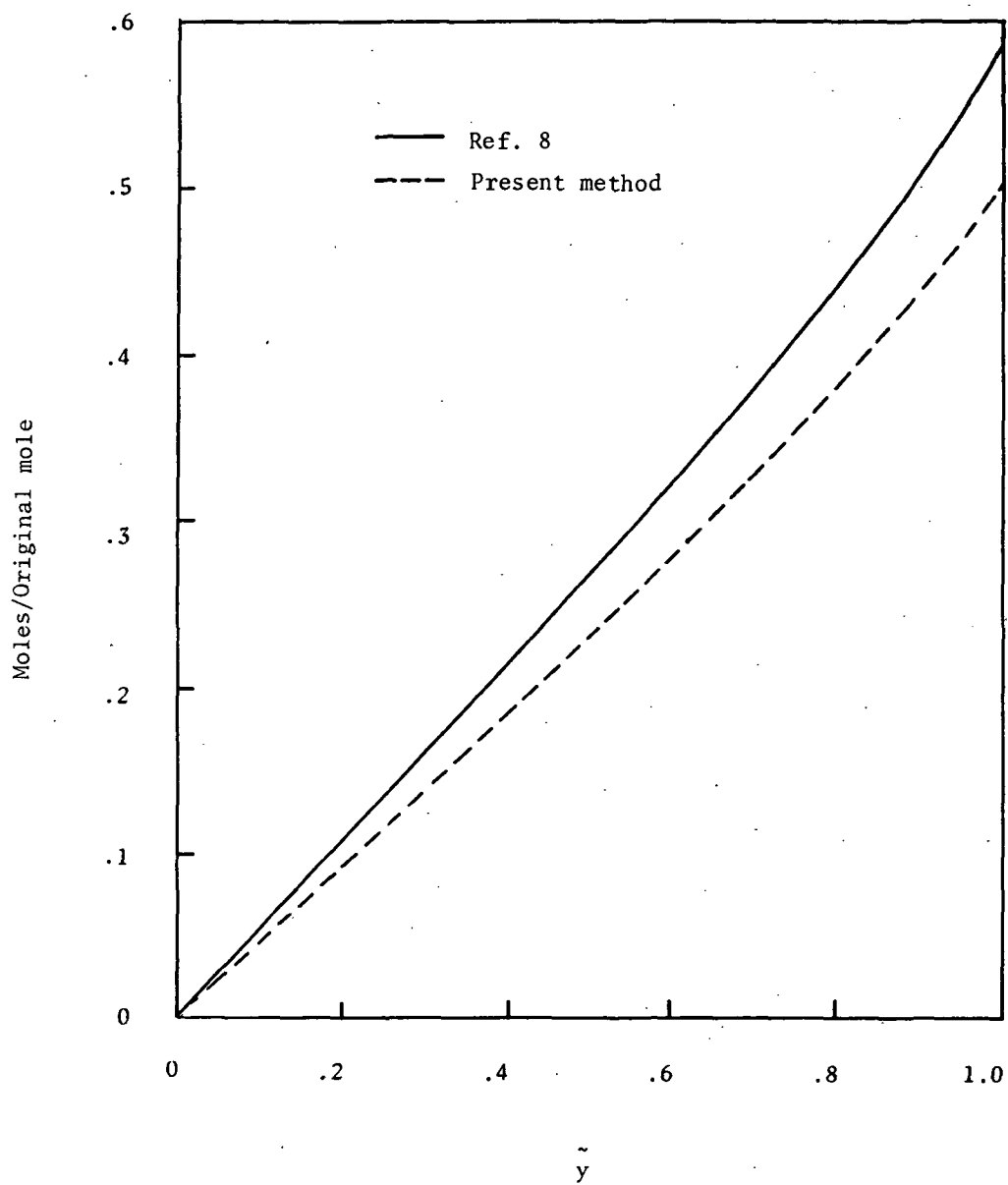


Figure 9.- Density variation across shock layer at $\theta = 81^\circ$. Case I.



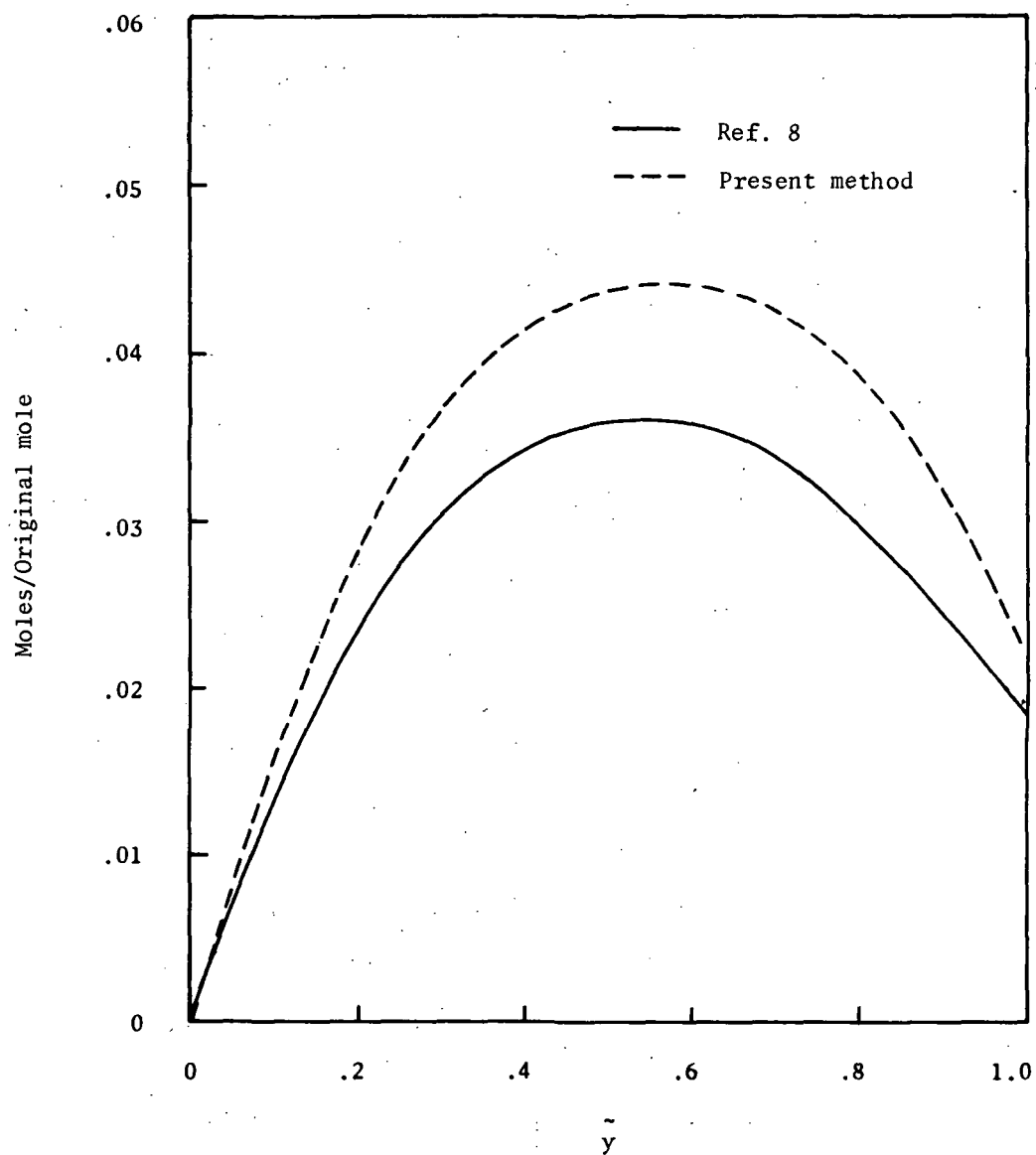
(a) Oxygen atom.

Figure 10.- Concentration variation across shock layer at $\theta = 81^\circ$. Case I.



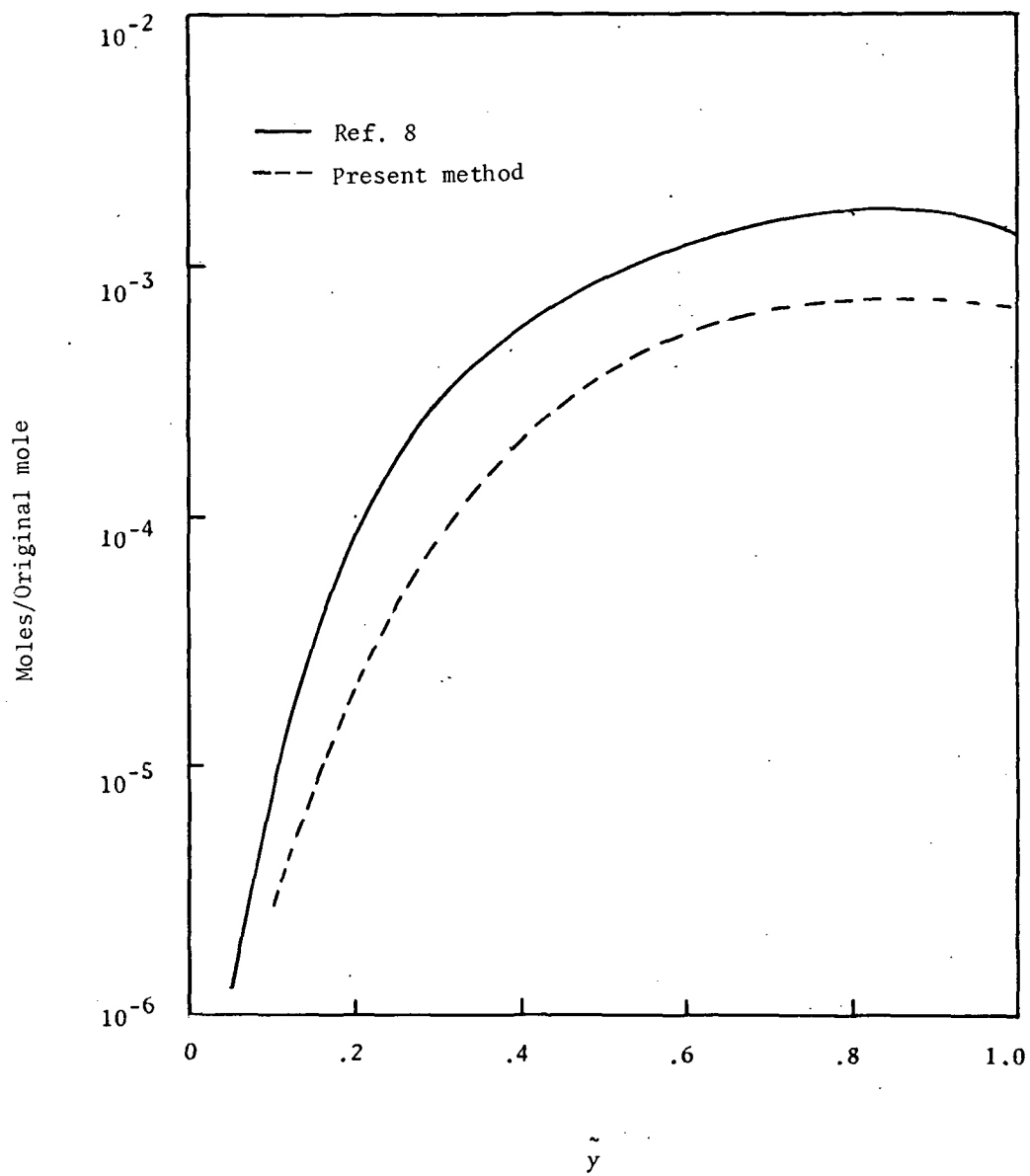
(b) Nitrogen atom.

Figure 10.- Continued.



(c) NO.

Figure 10.- Continued.



(d) Electron.

Figure 10.- Concluded.

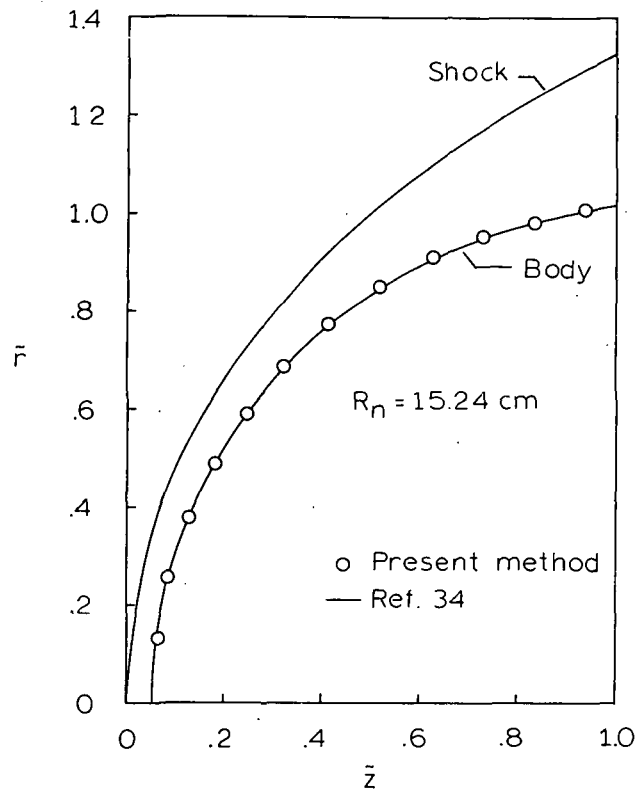


Figure 11.- Assumed shock and computed body shape. Case II.

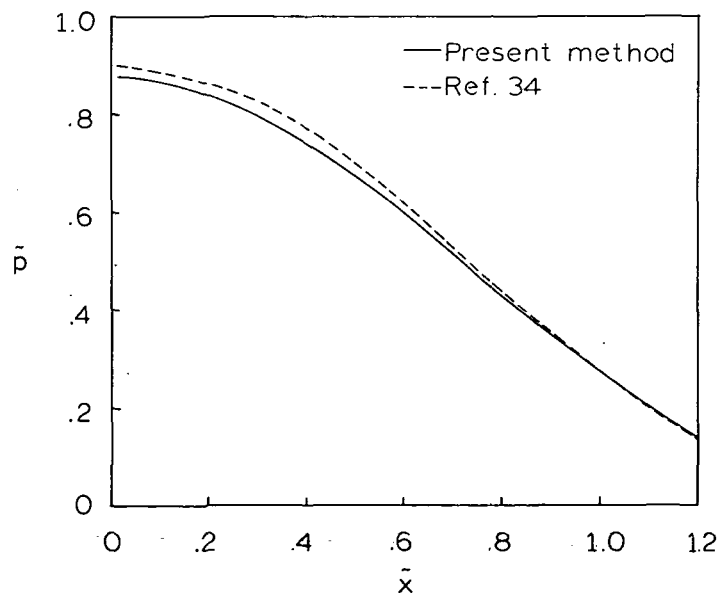


Figure 12.- Pressure variation along body surface. Case II.

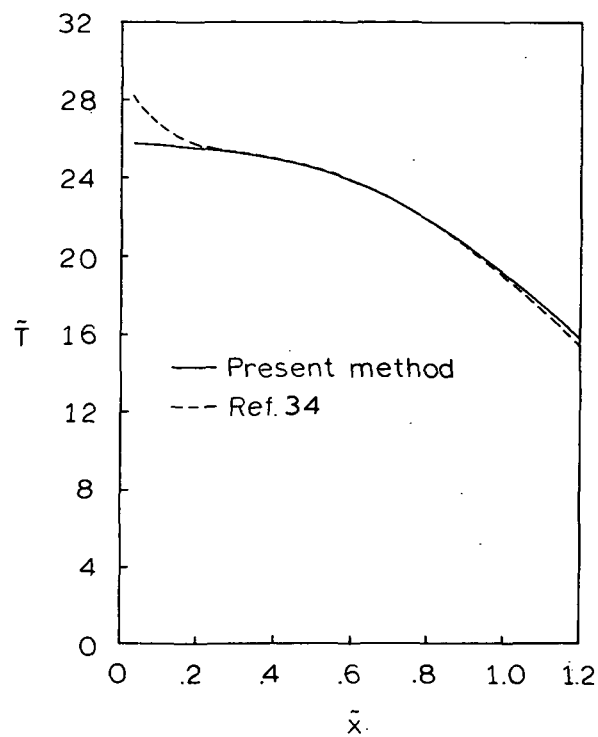


Figure 13.- Temperature variation along body surface. Case II.

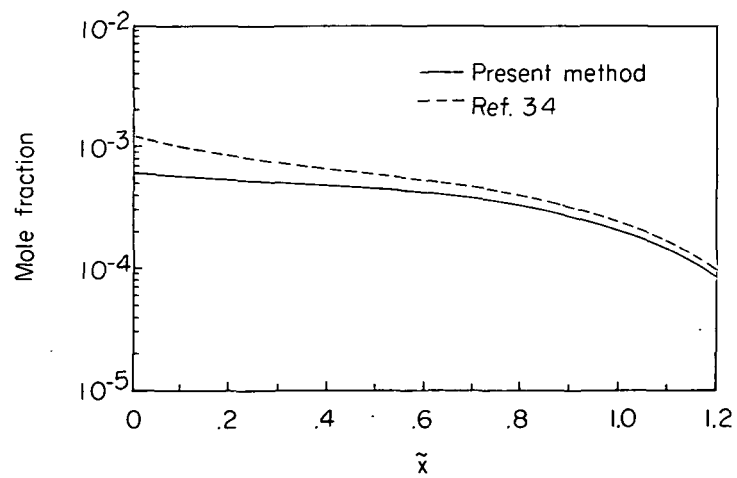


Figure 14.- Electron concentration along body surface. Case II.

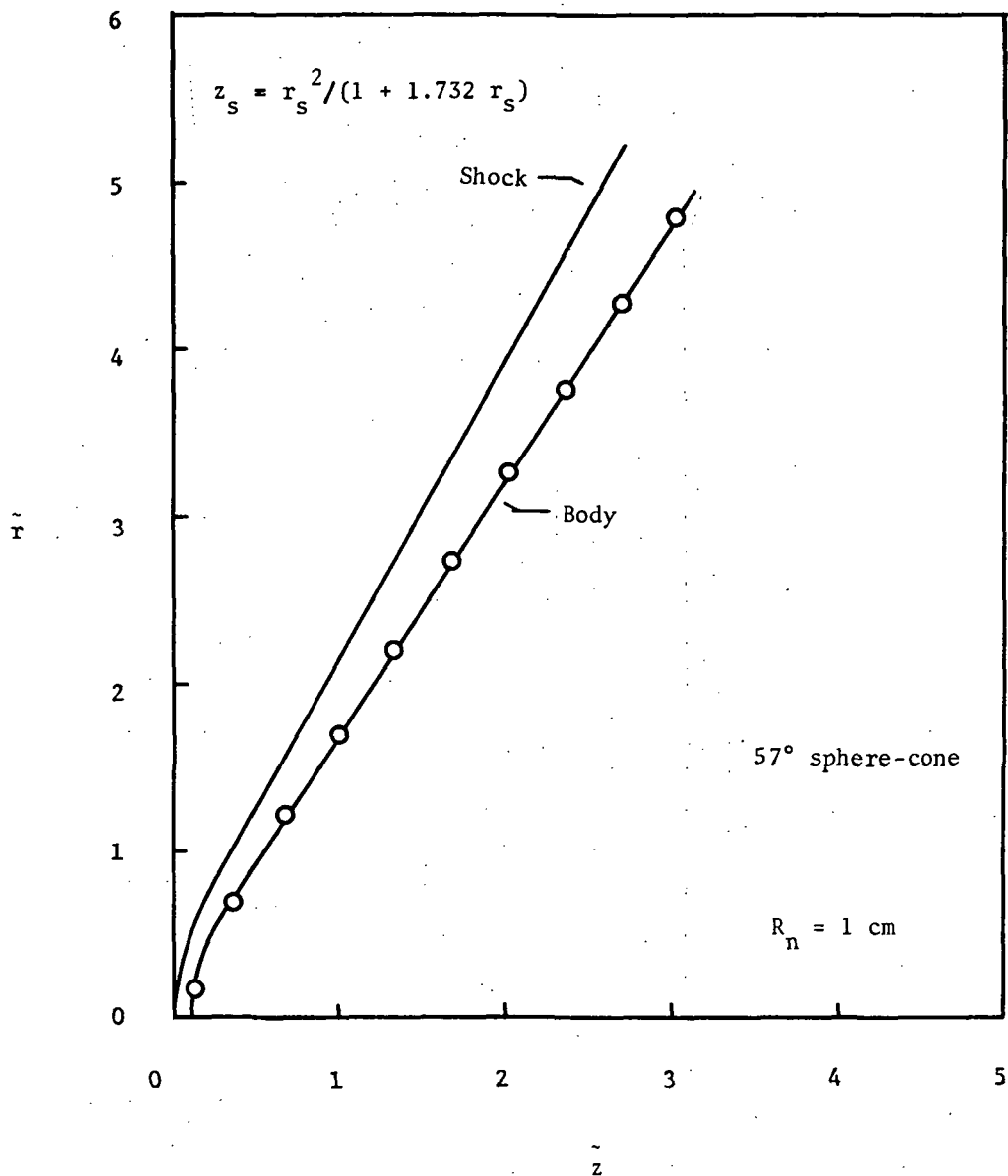


Figure 15.- Assumed shock and computed body shape. Case III.

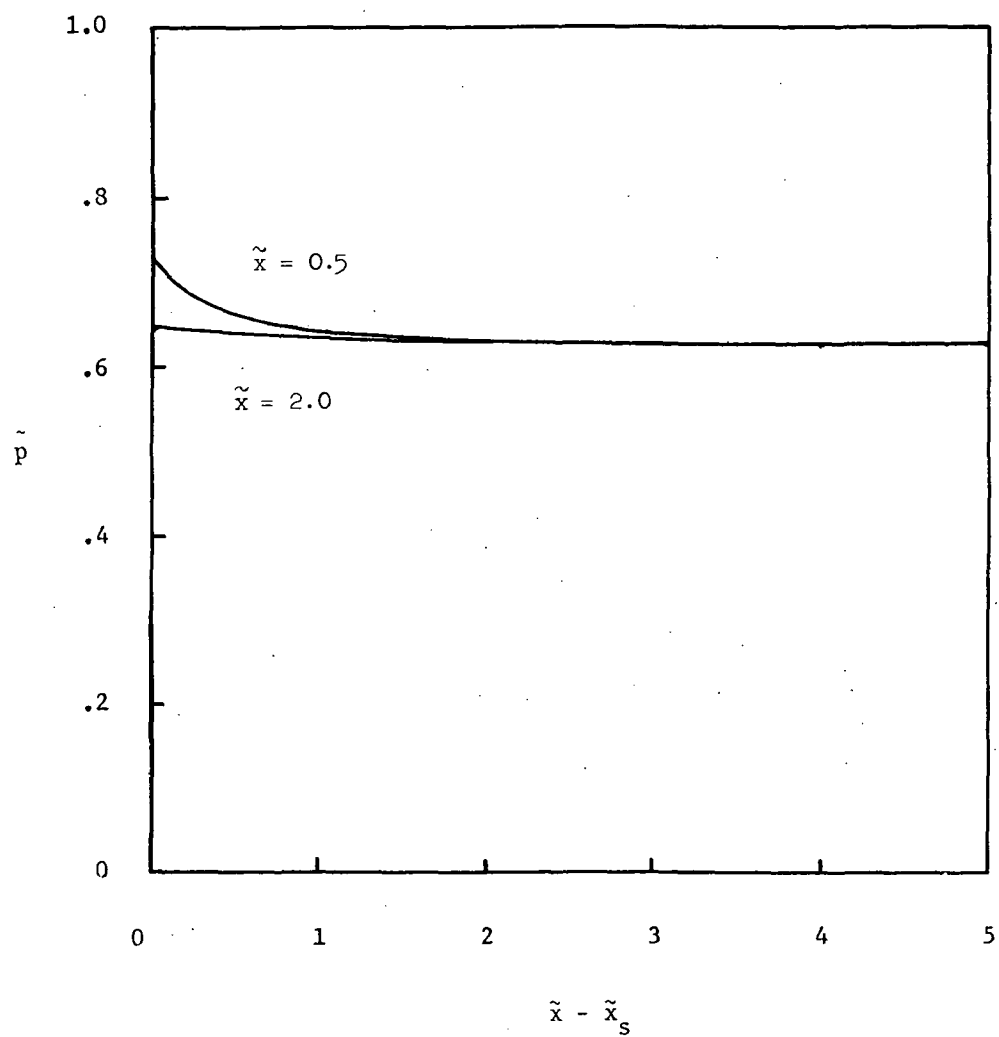


Figure 16.- Pressure variation along streamlines crossing the shock at $\tilde{x} = 0.5$ and $\tilde{x} = 2.0$. Case III.

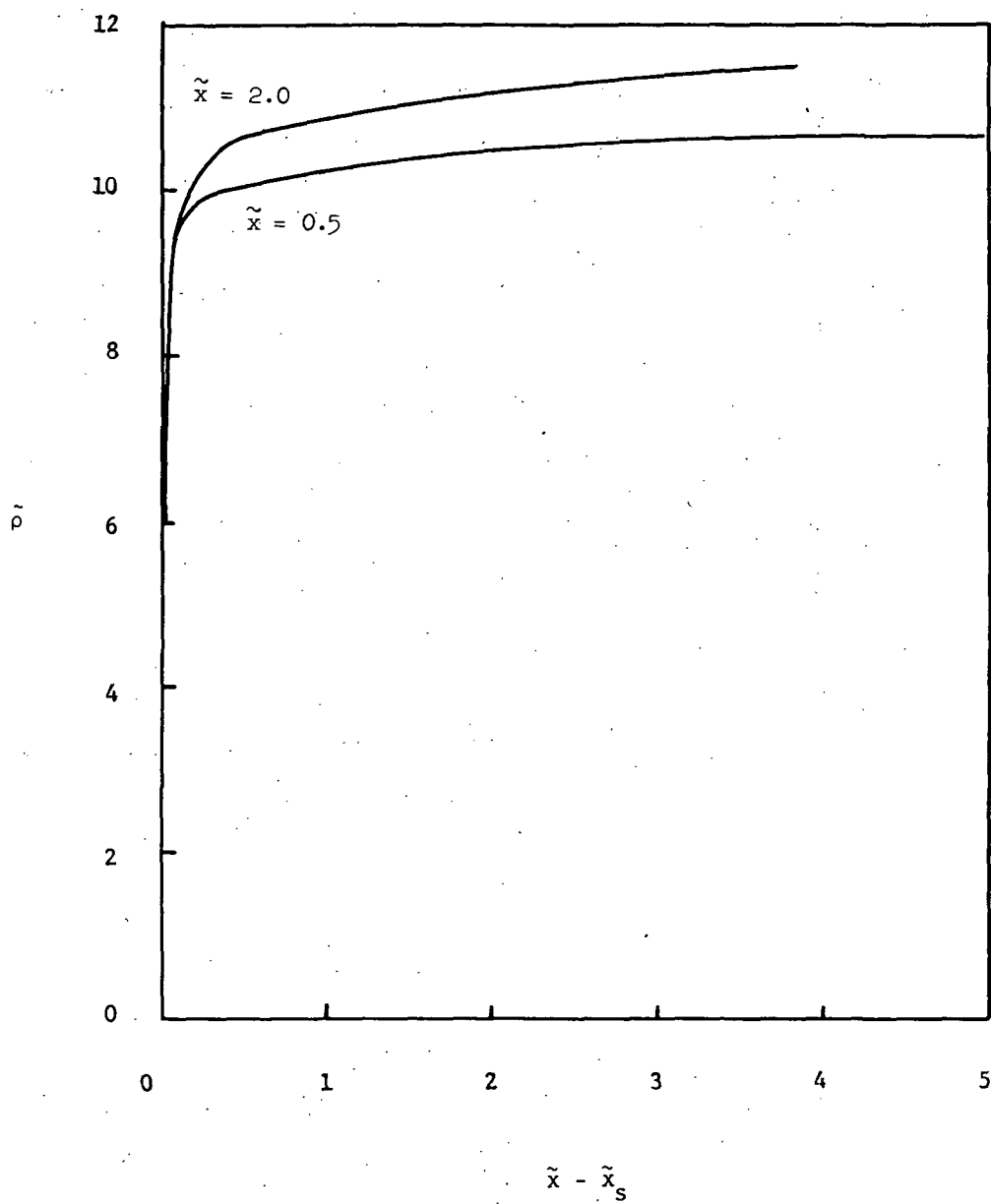


Figure 17.- Density variation along streamlines crossing the shock at $\tilde{x} = 0.5$ and $\tilde{x} = 2.0$. Case III.

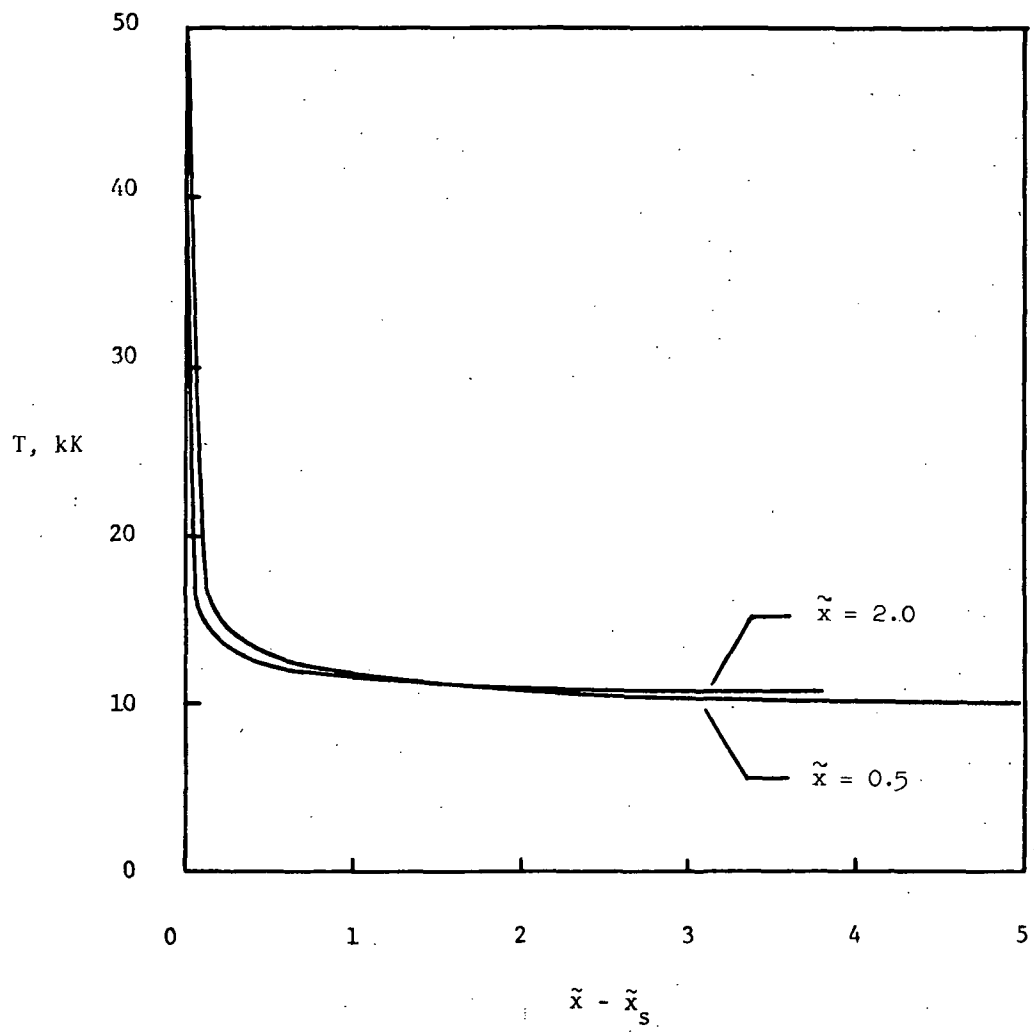
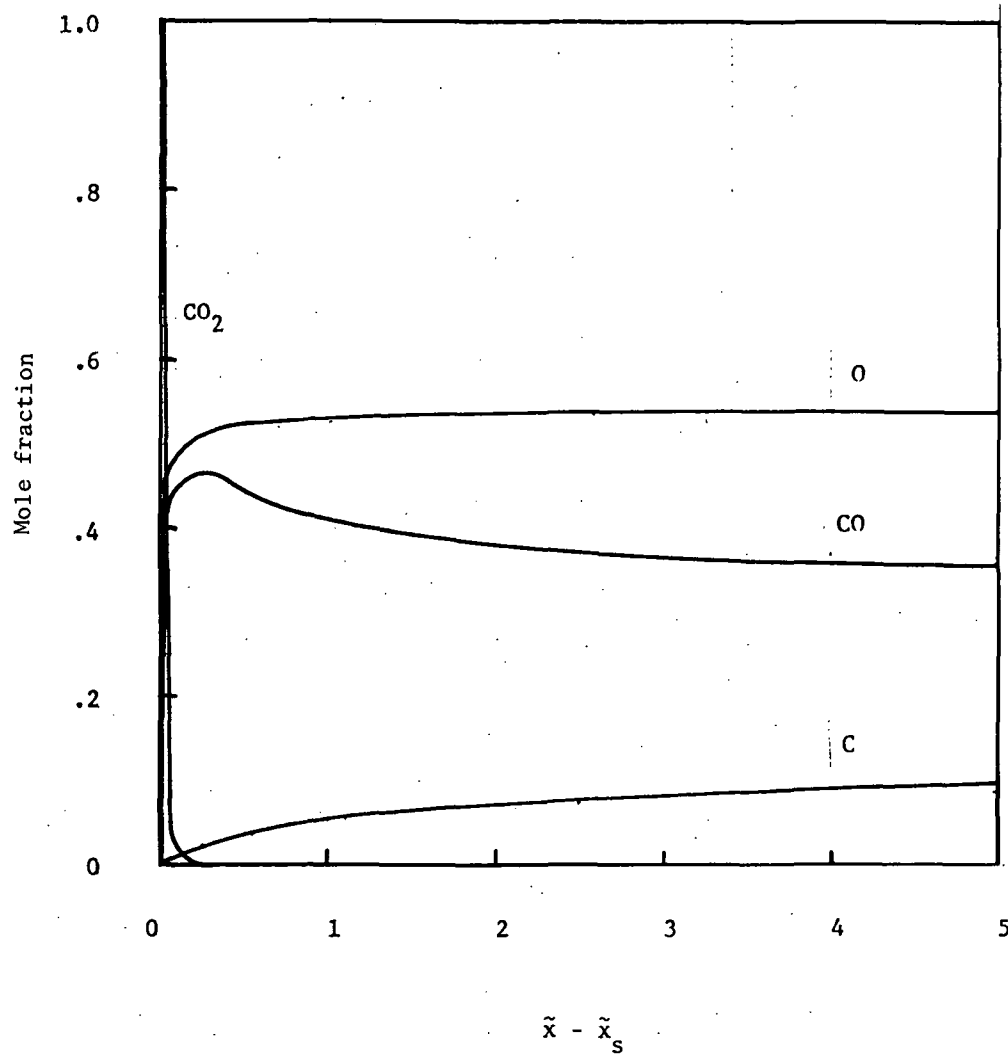
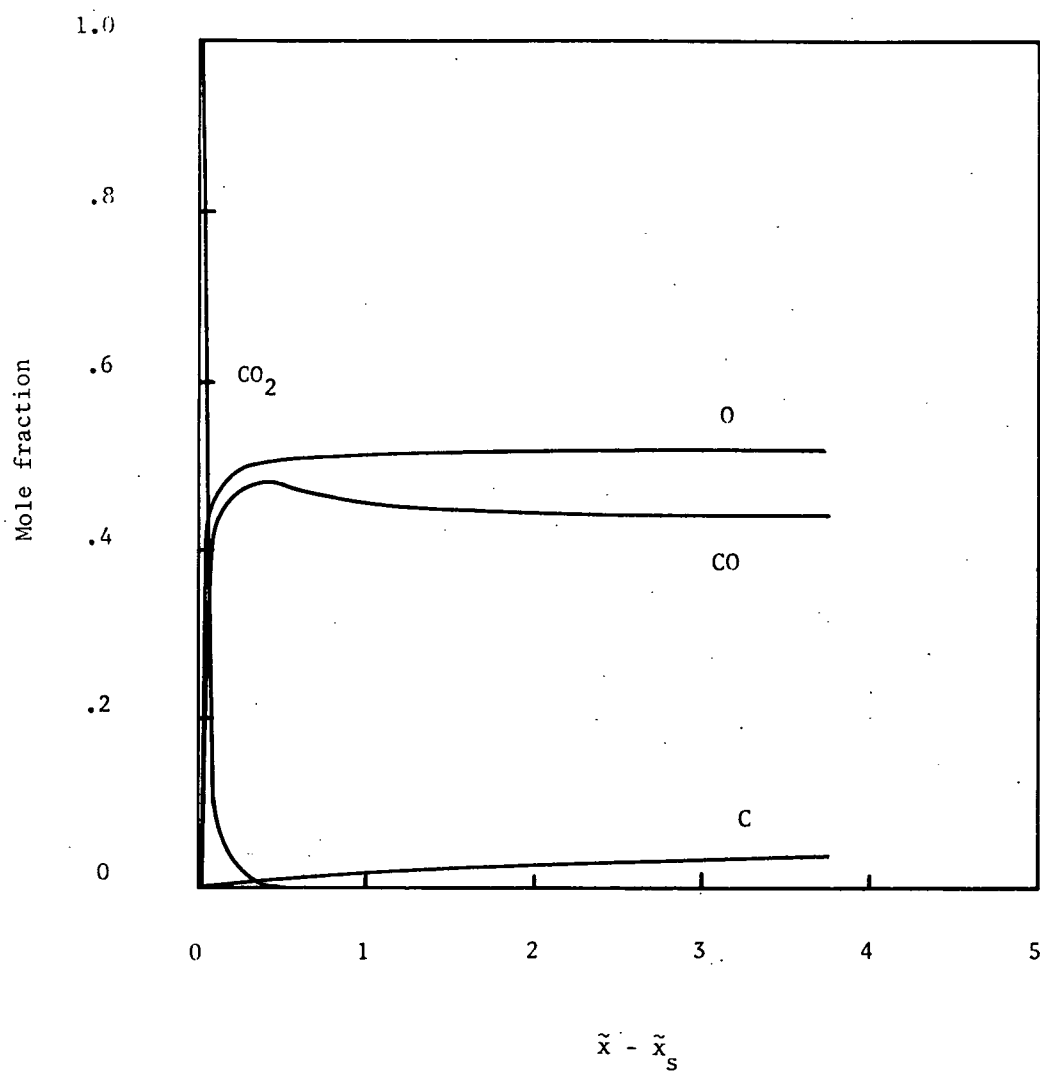


Figure 18.- Temperature variation along streamlines crossing the shock at $\tilde{x} = 0.5$ and $\tilde{x} = 2.0$. Case III.



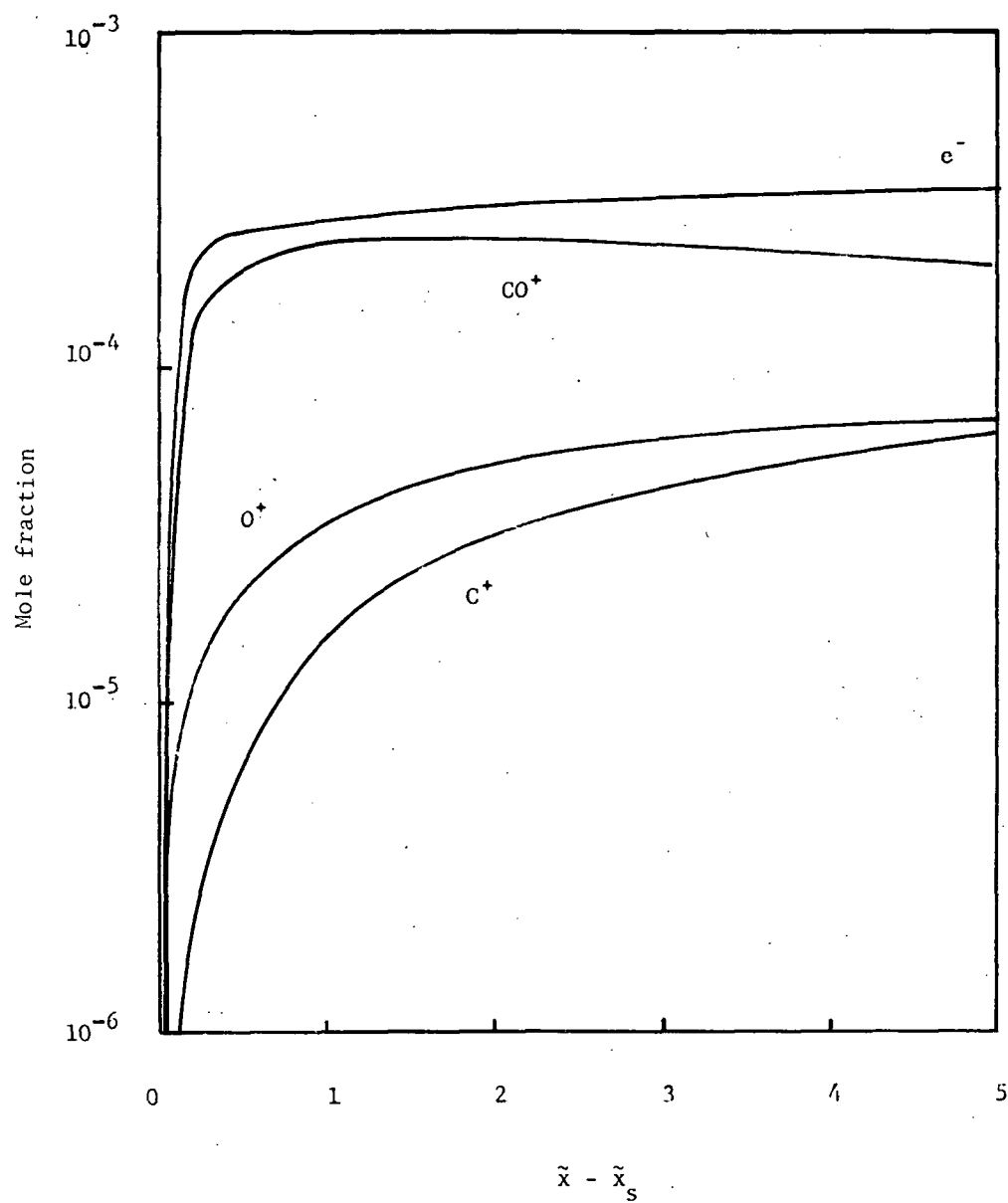
(a) $\tilde{x} = 0.5$; O , CO , C , CO_2 .

Figure 19.- Species concentrations along streamline crossing the shock. Case III.



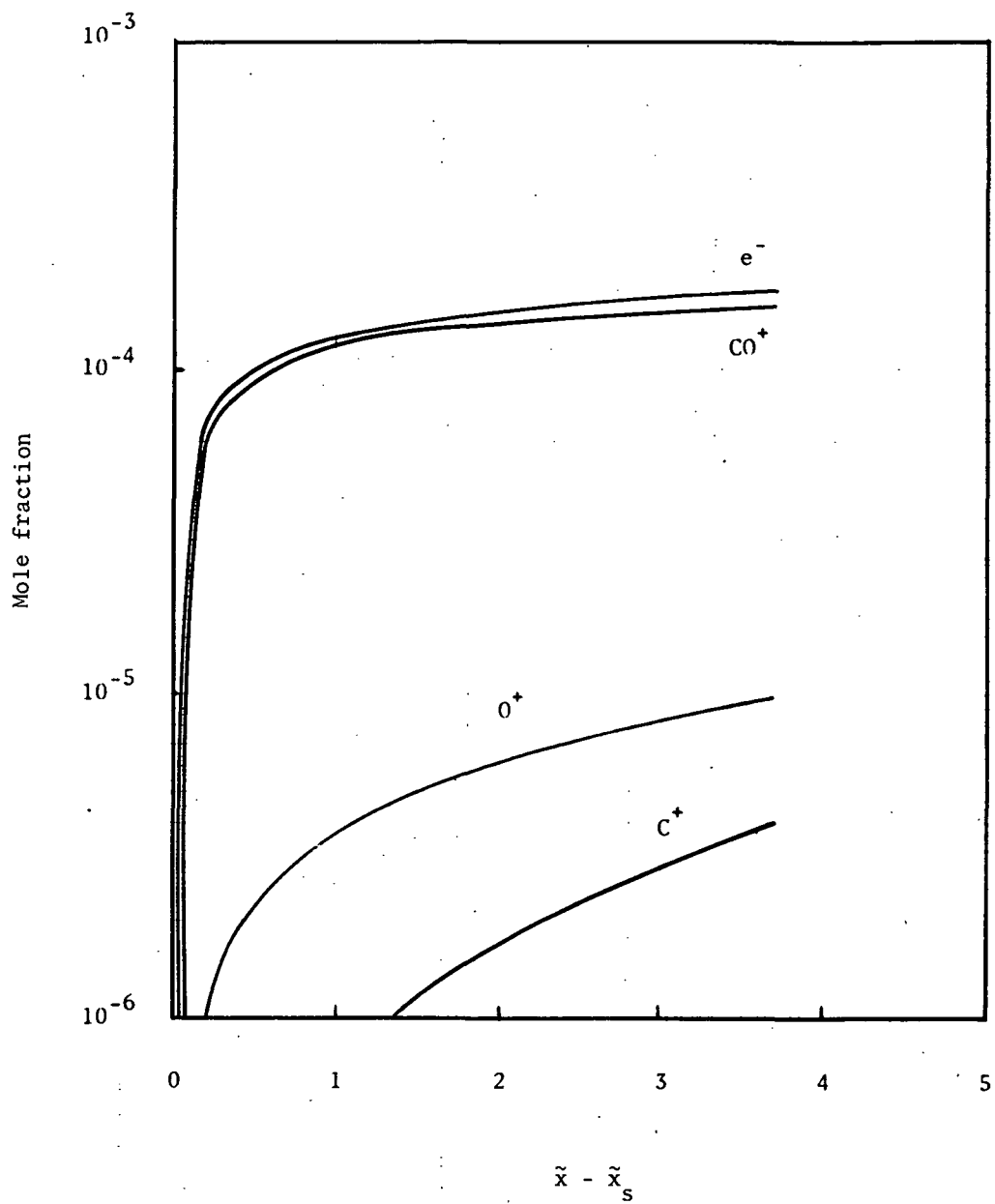
(b) $\tilde{x} = 2.0$; O, CO, C, CO_2 .

Figure 19.- Continued.



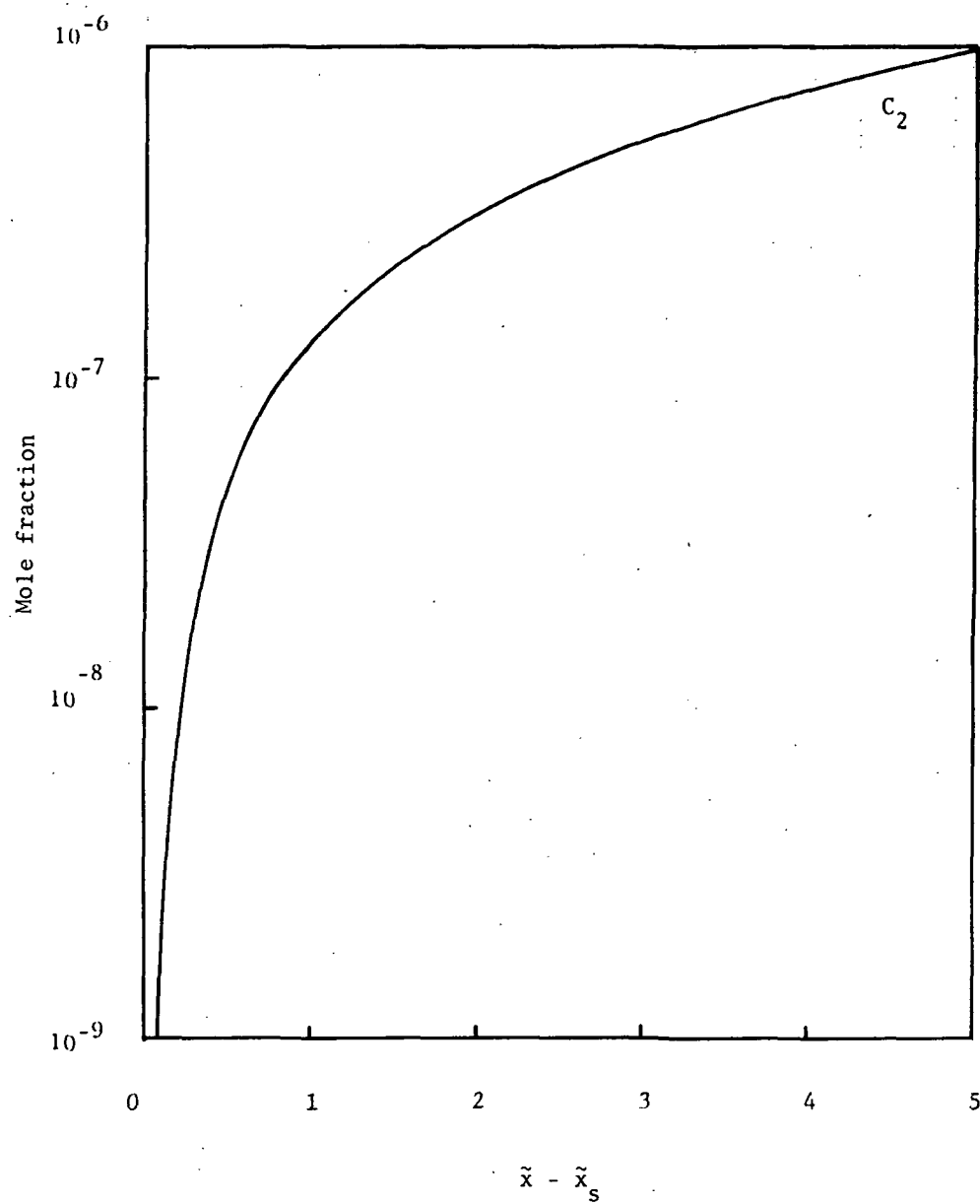
(c) $\tilde{x} = 0.5$; e^- , CO^+ , O^+ , C^+ .

Figure 19.- Continued.



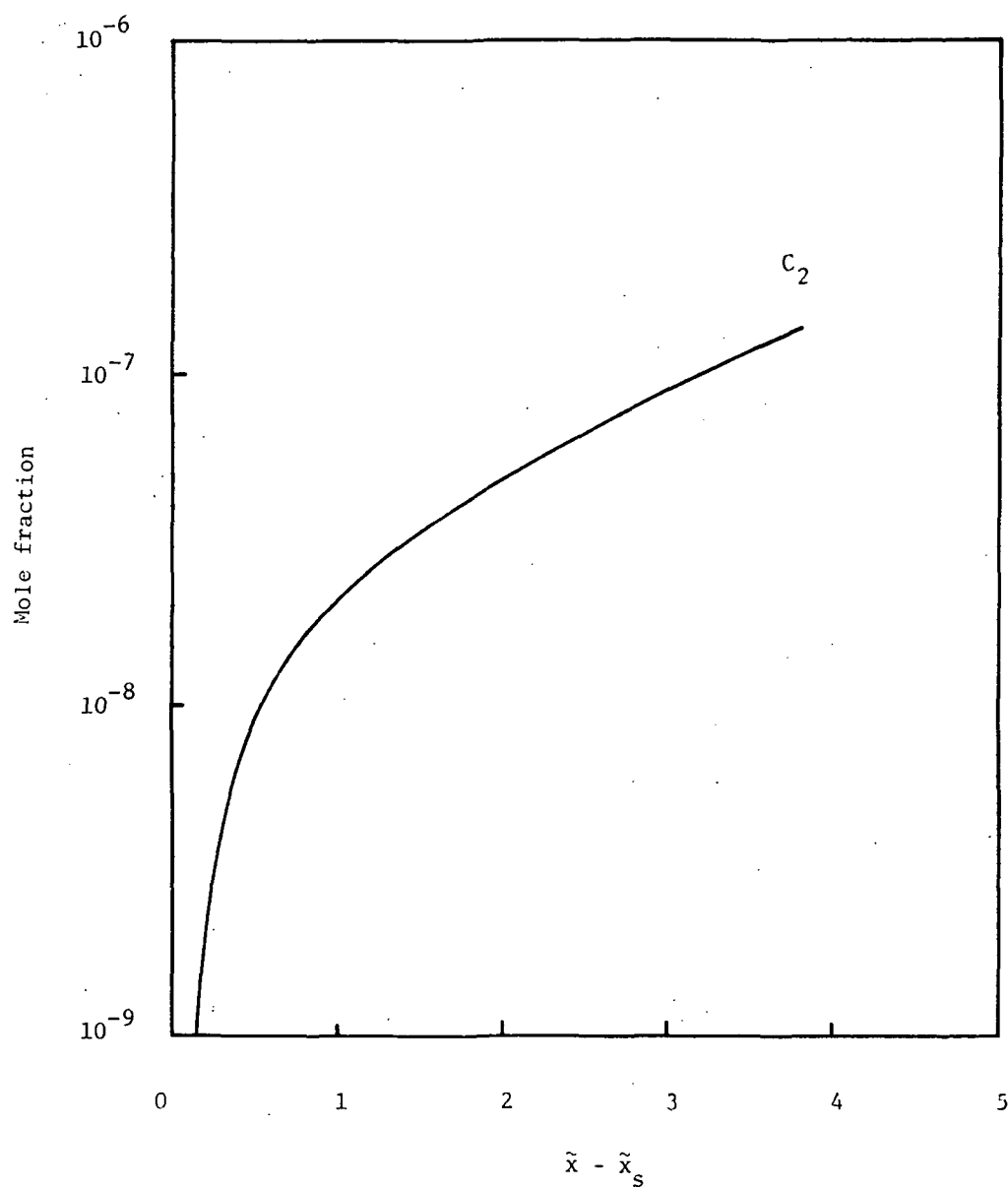
(d) $\tilde{x} = 2.0$; e^- , CO^+ , O^+ , C^+ .

Figure 19.- Continued.



(e) $\tilde{x} = 0.5$; C_2 .

Figure 19.- Continued.



(f) $\tilde{x} = 2.0$; C_2 .

Figure 19.- Concluded.

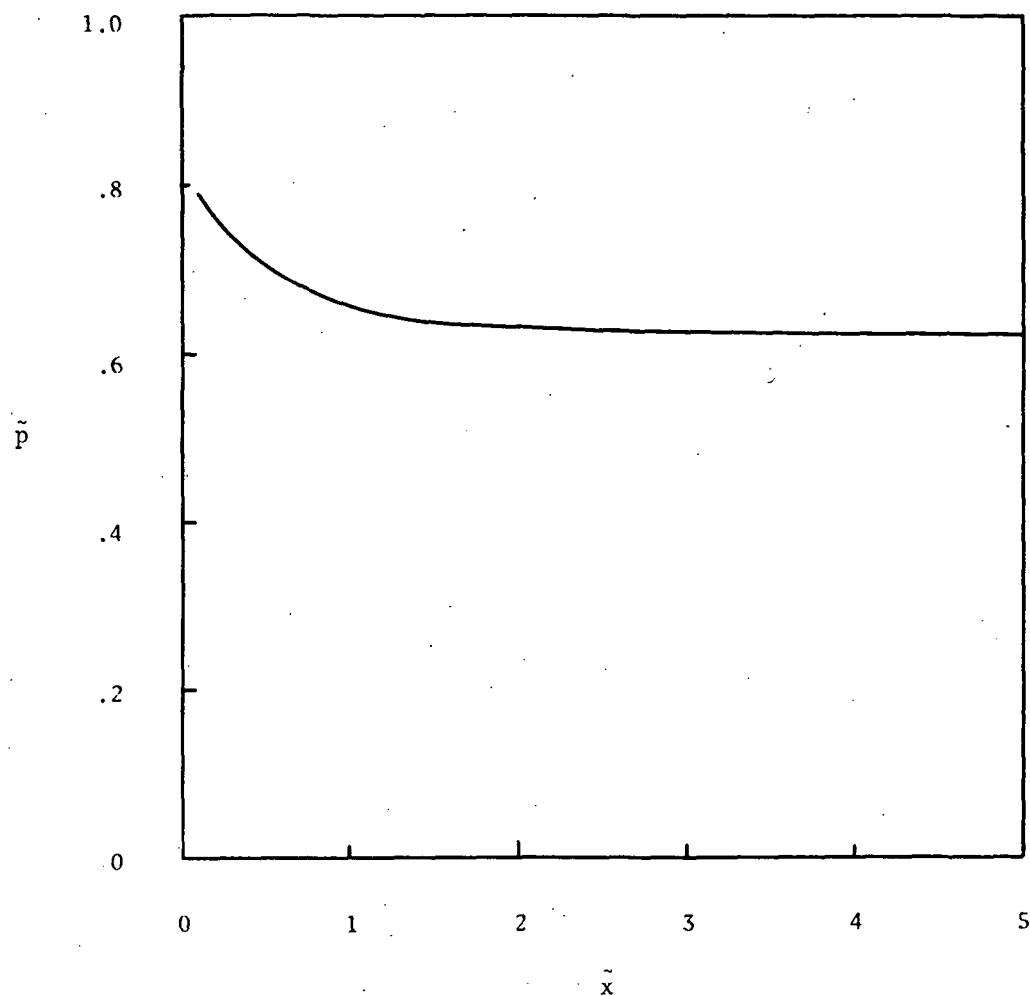


Figure 20.- Pressure distribution along surface of body. Case III.

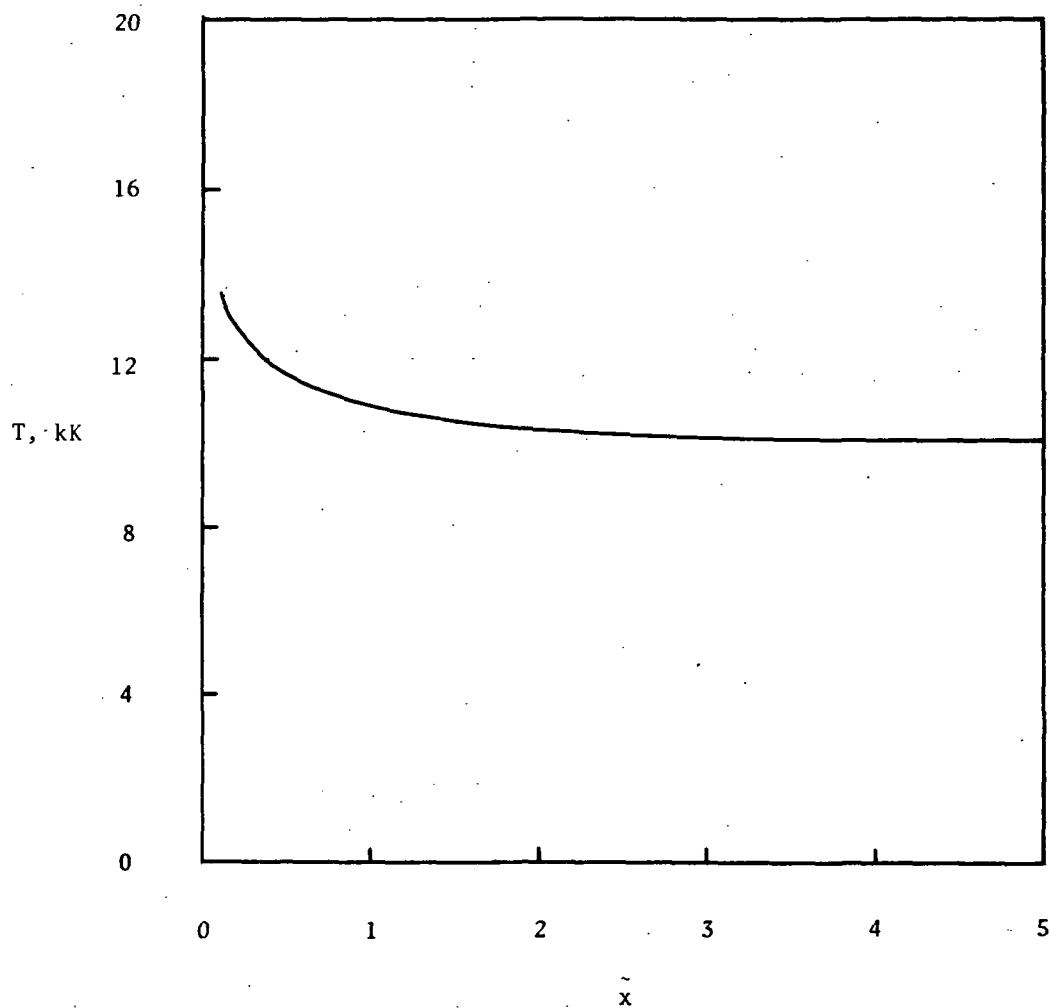
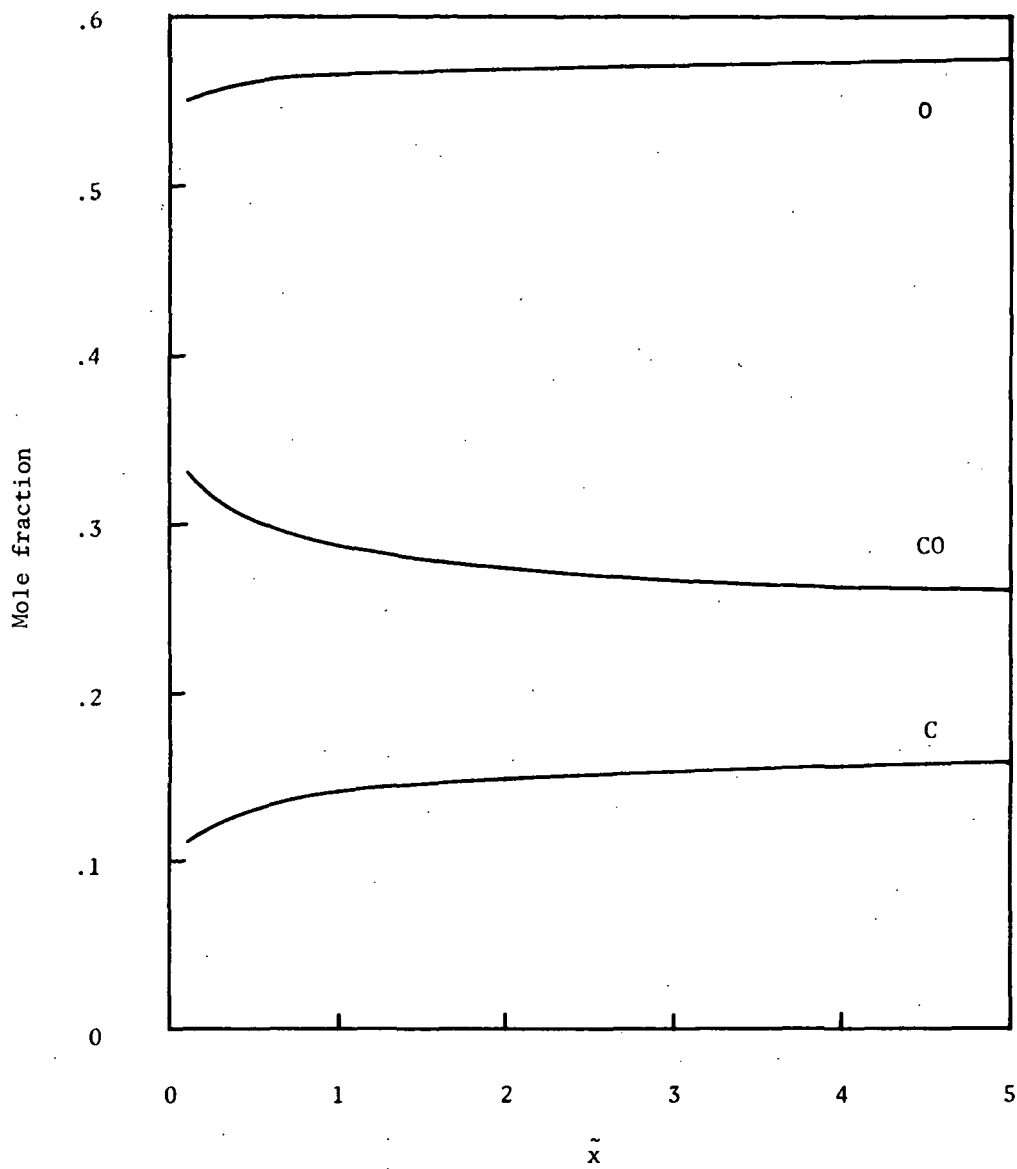
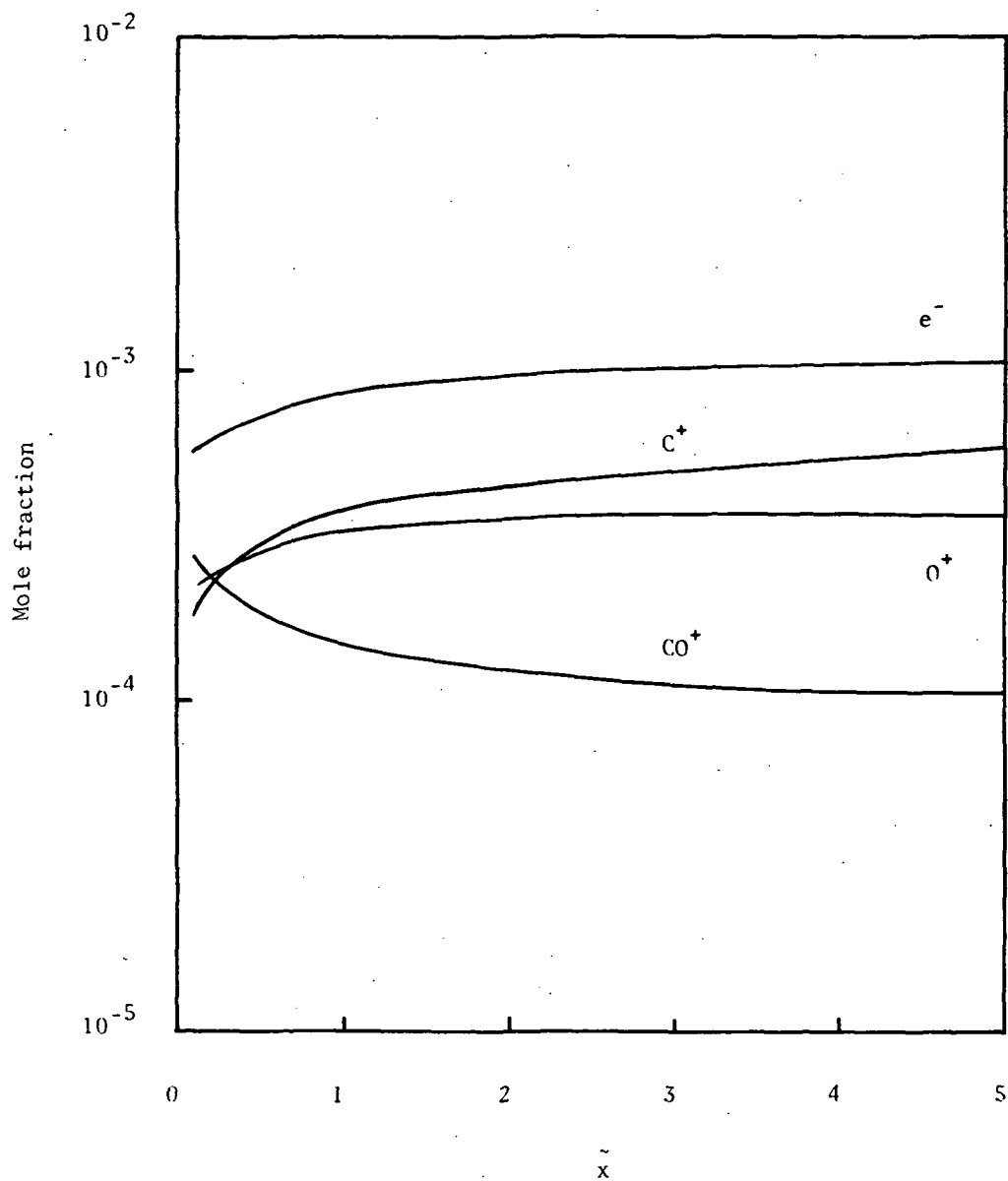


Figure 21.- Temperature distribution along surface of body. Case III.



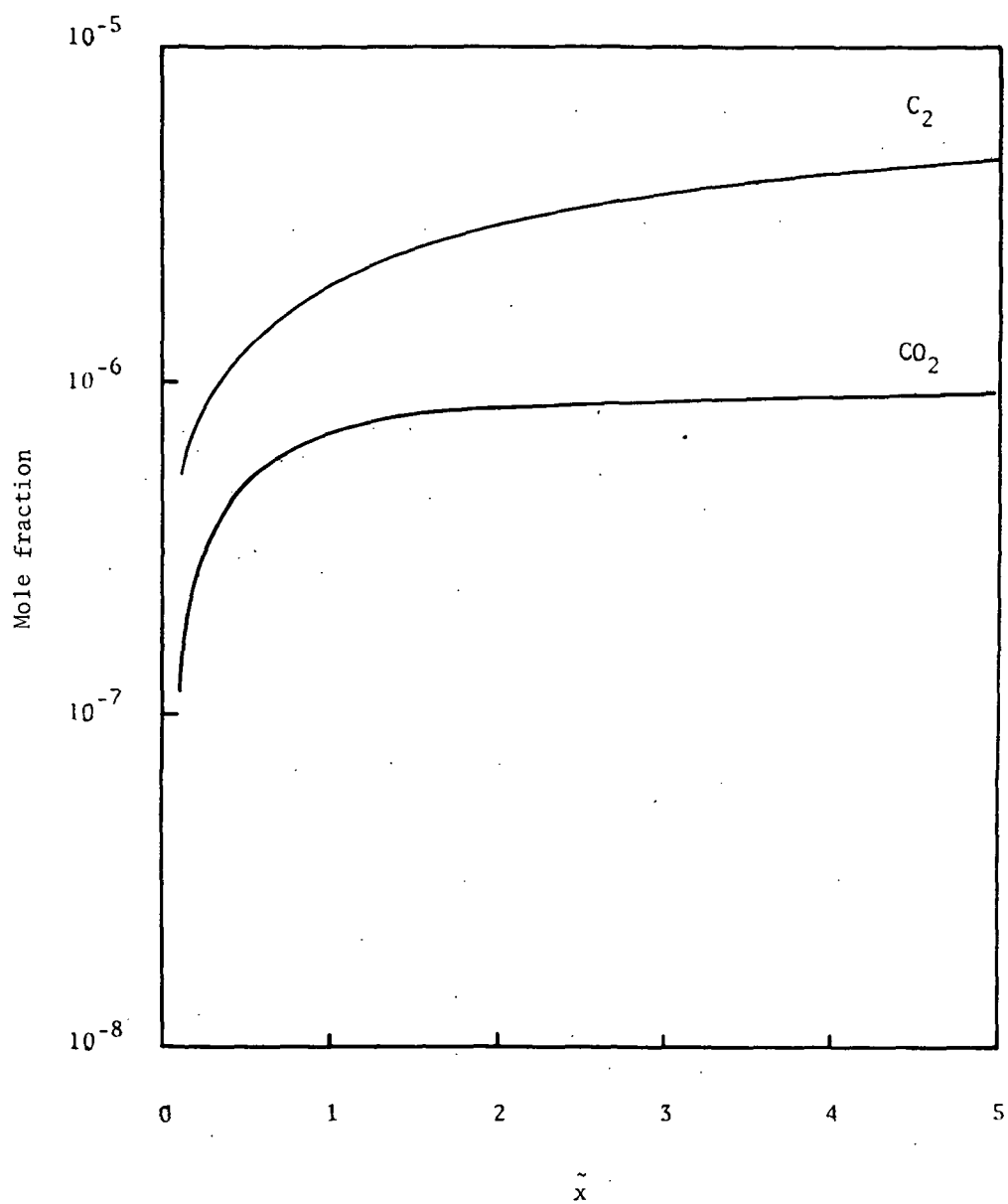
(a) O, CO, and C.

Figure 22.- Species concentrations along surface of body. Case III.



(b) e^- , C^+ , O^+ , and CO^+ .

Figure 22.- Continued.



(c) C_2 and CO_2 .

Figure 22.- Concluded.

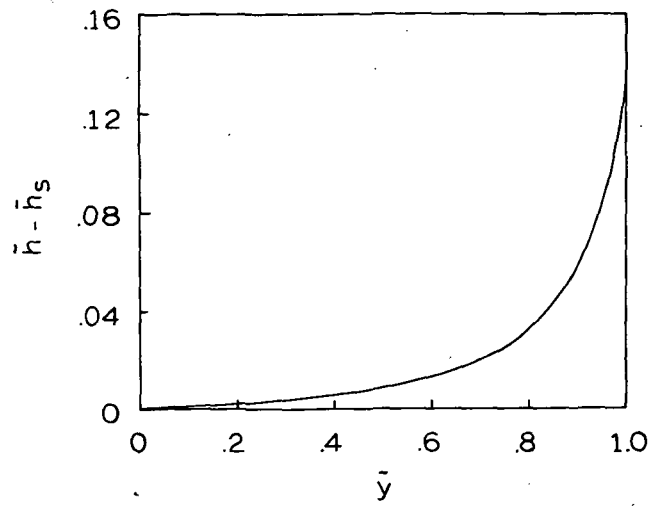


Figure 23.- Static enthalpy profile across shock layer at $\tilde{x} = 2.0$. Case III.

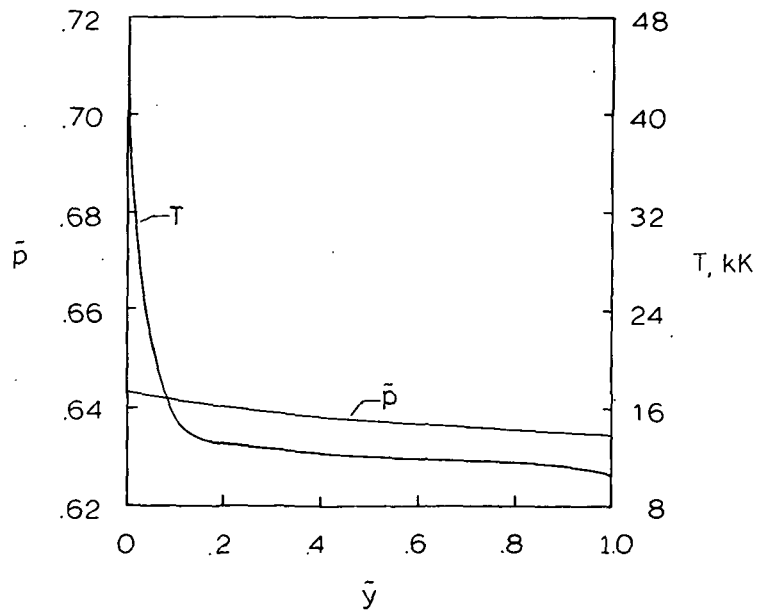


Figure 24.- Pressure and temperature profiles across shock layer at $\tilde{x} = 2.0$. Case III.

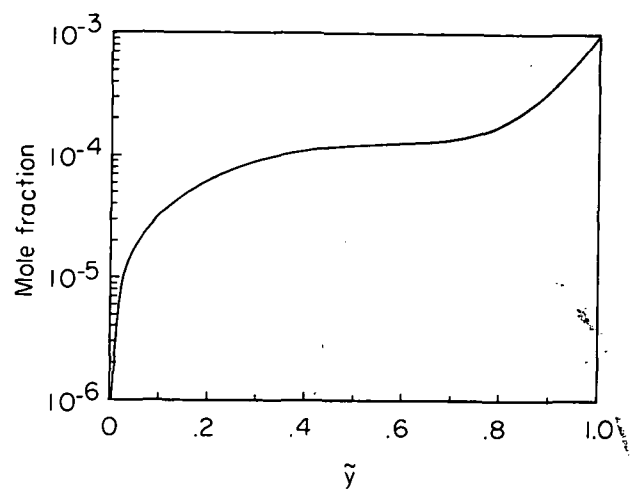


Figure 25.- Electron concentration profiles across shock layer at $\tilde{x} = 2.0$. Case III.

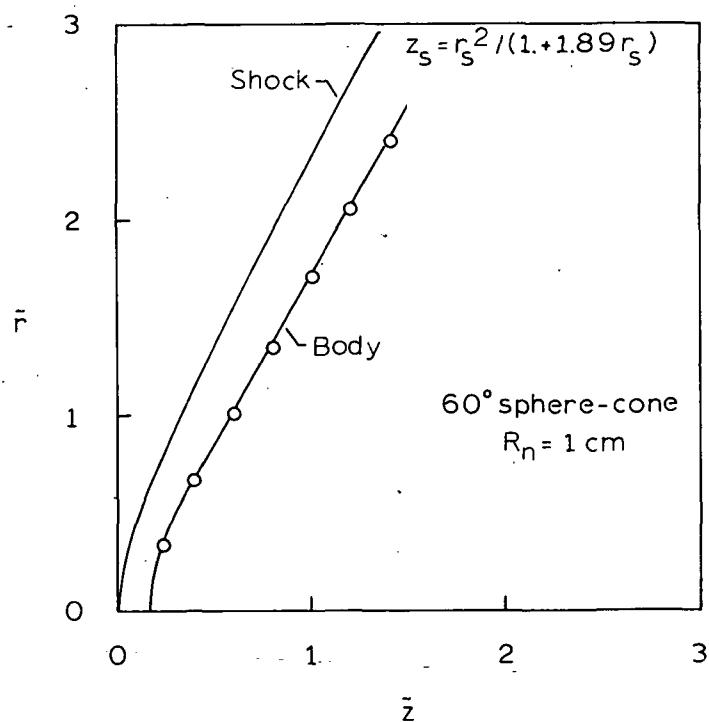


Figure 26.- Assumed shock and computed body shape. Case IV.

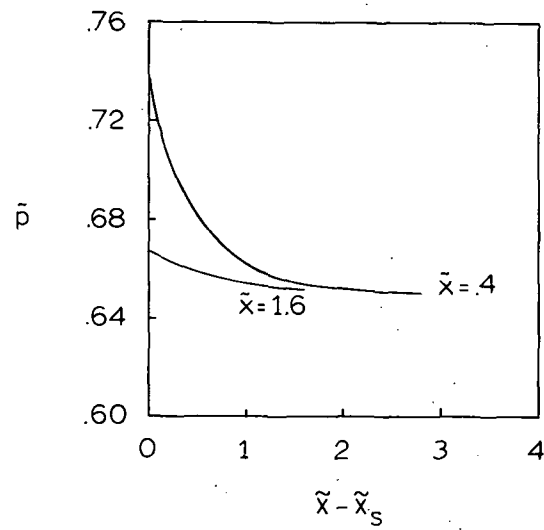


Figure 27.- Pressure variation along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6. Case IV.

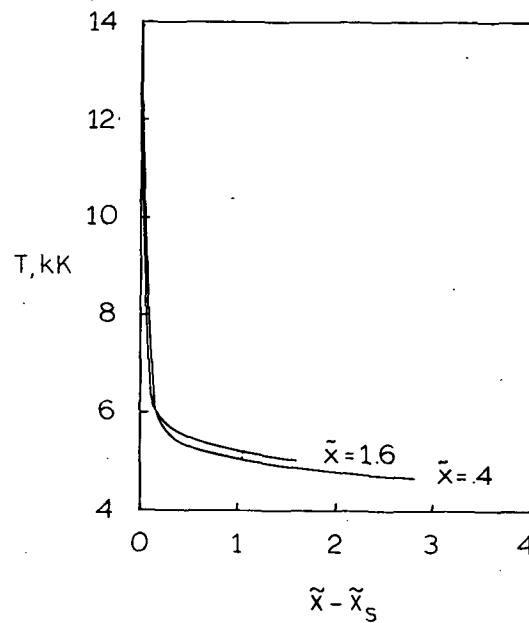
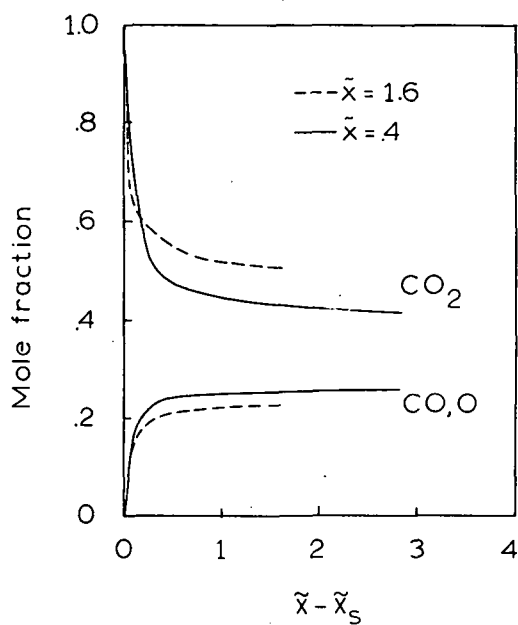
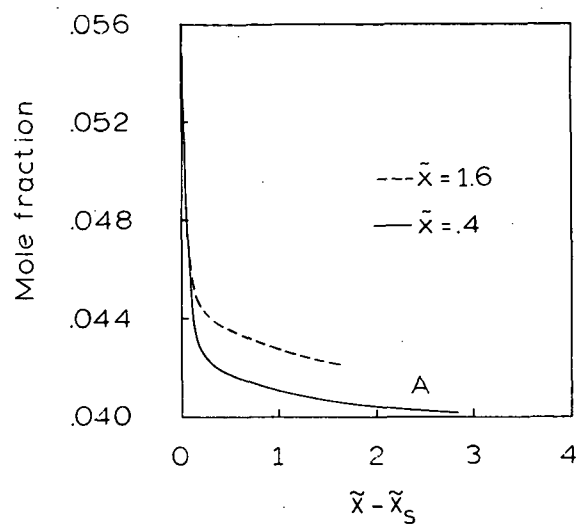


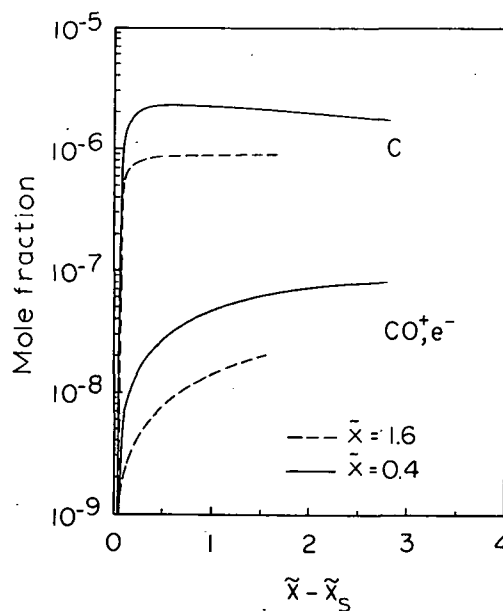
Figure 28.- Temperature variation along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6. Case IV.



(a) CO_2 , CO , and O .



(b) A.



(c) C , CO^+ , and e^- .

Figure 29.- Species concentrations along streamlines crossing the shock at $\tilde{x} = 0.4$ and $\tilde{x} = 1.6$. Case IV.

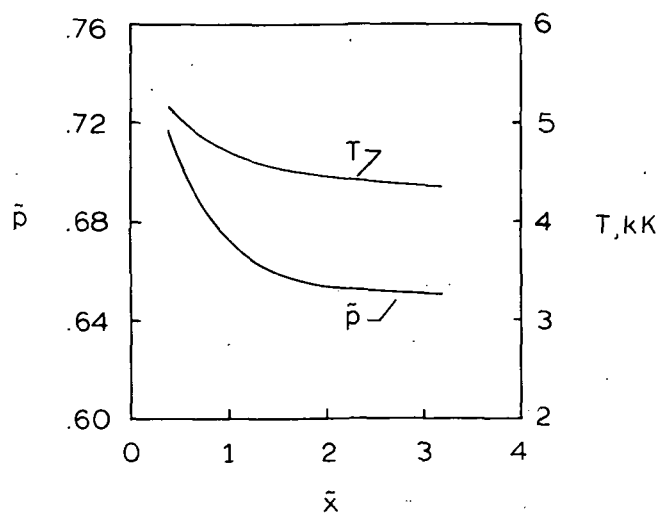
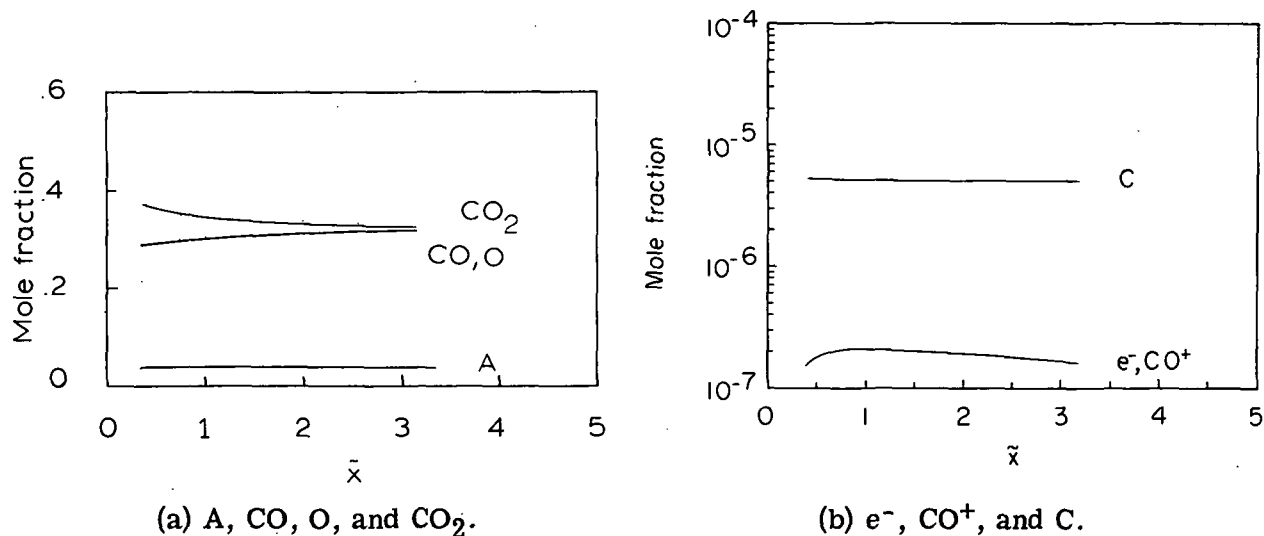


Figure 30.- Pressure and temperature variations along body surface. Case IV.



(a) A , CO , O , and CO_2 .

(b) e^- , CO^+ , and C .

Figure 31.- Species concentrations along body surface. Case IV.

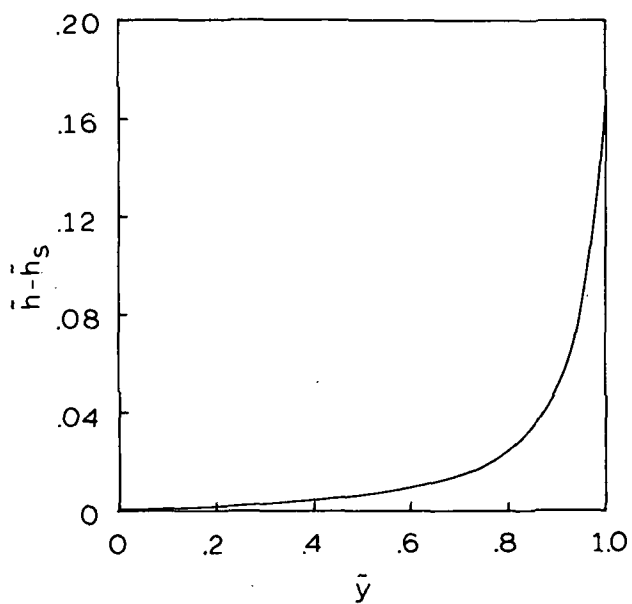


Figure 32.- Static enthalpy profile across shock layer at $\tilde{x} = 1.6$. Case IV.

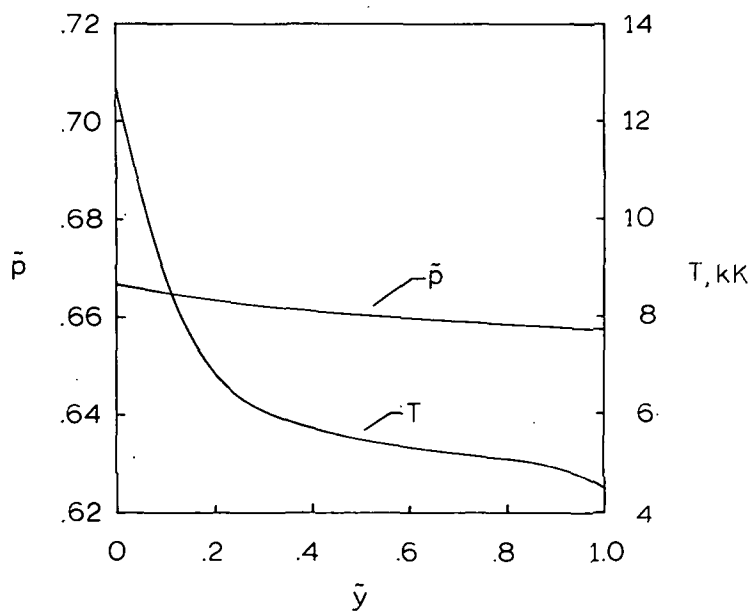


Figure 33.- Pressure and temperature profiles across shock layer at $\tilde{x} = 1.6$. Case IV.

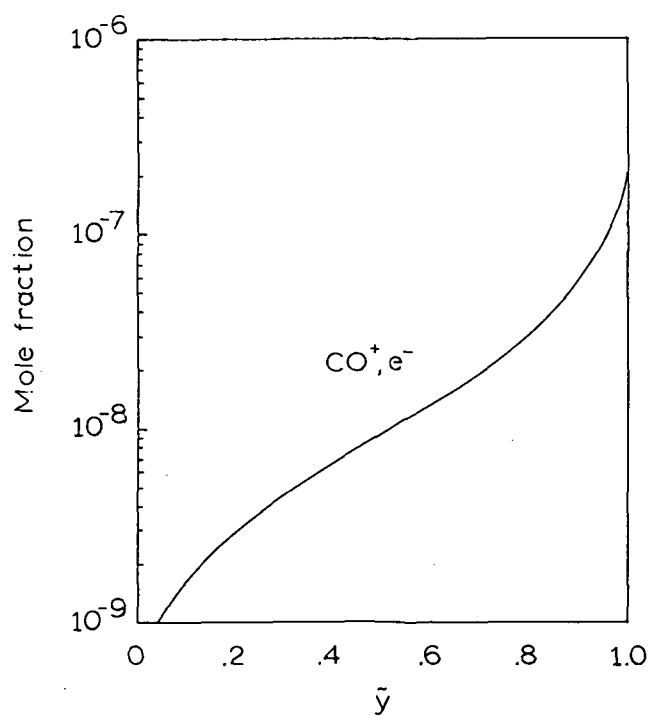


Figure 34.- Electron concentration profile across shock layer at $\tilde{x} = 1.6$. Case IV.

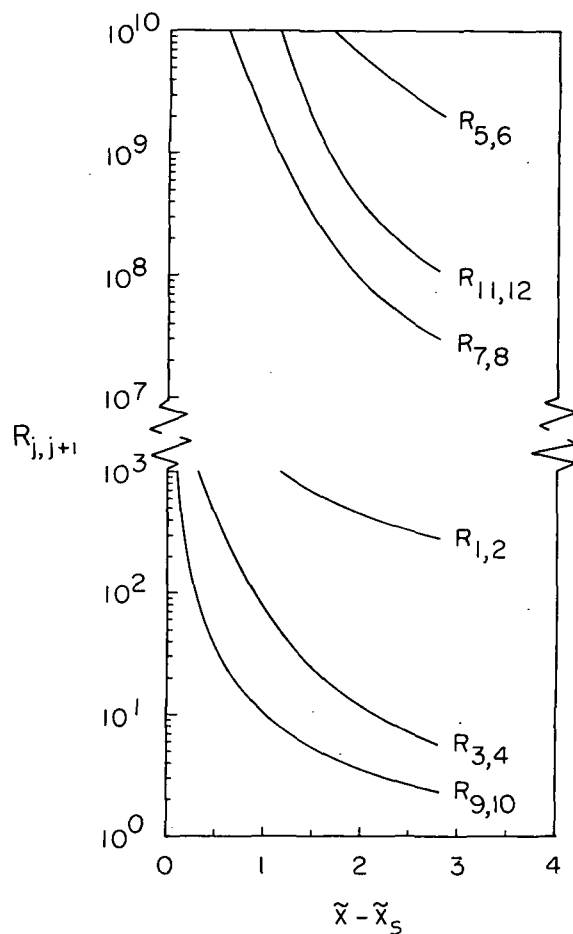


Figure 35.- Ratio of forward reaction rate to reverse reaction rate along inner streamline ($\tilde{x} = 0.4$). Case IV.

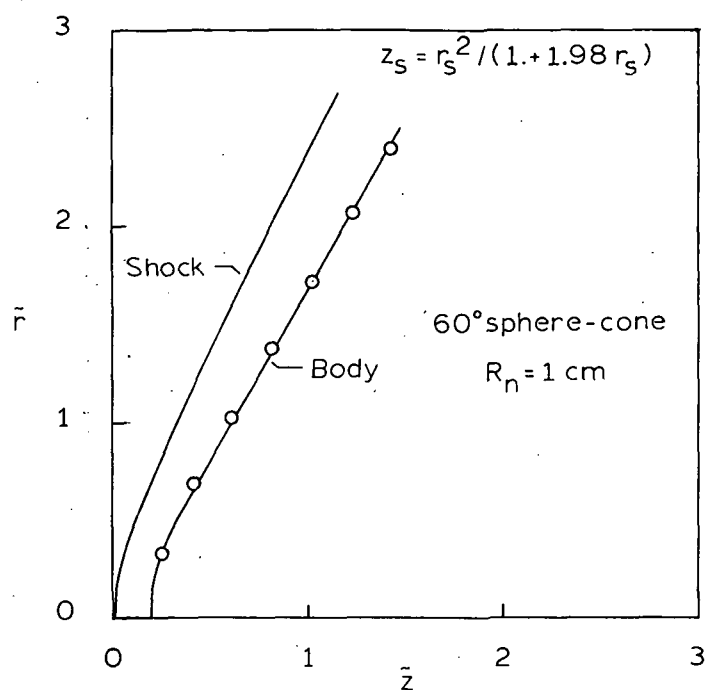


Figure 36.- Assumed shock shape and computed body shape. Case V.

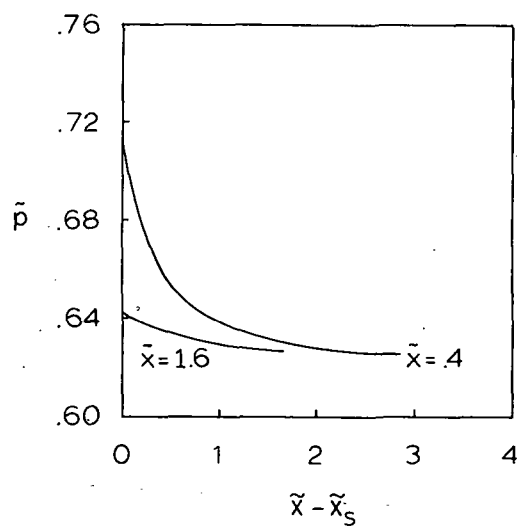


Figure 37.- Pressure variations along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6 . Case V.

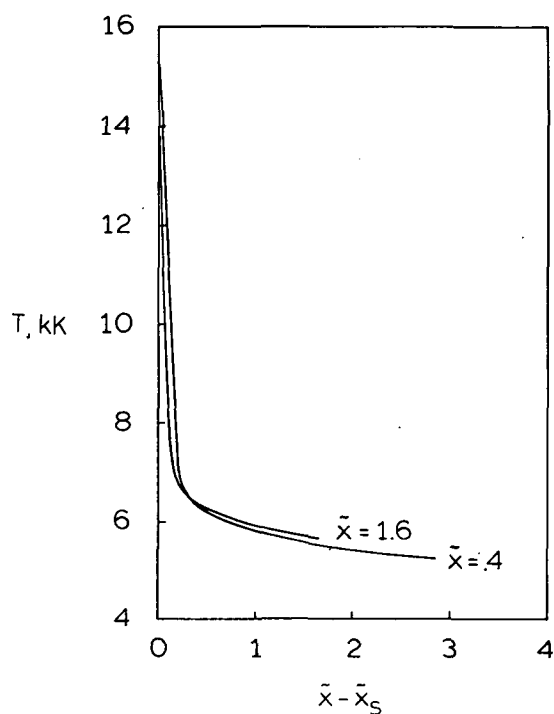
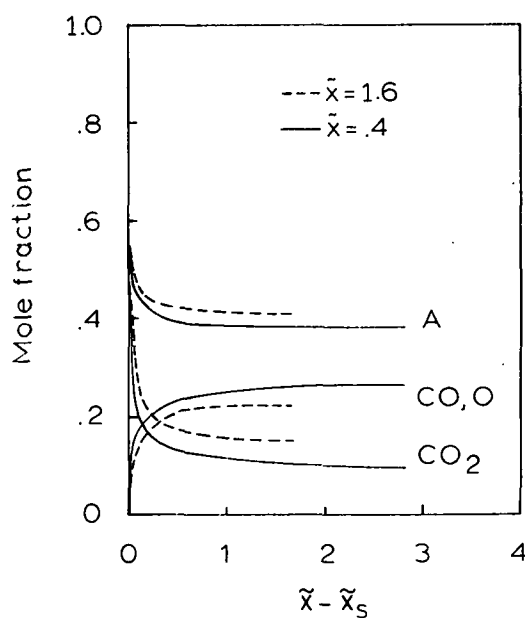
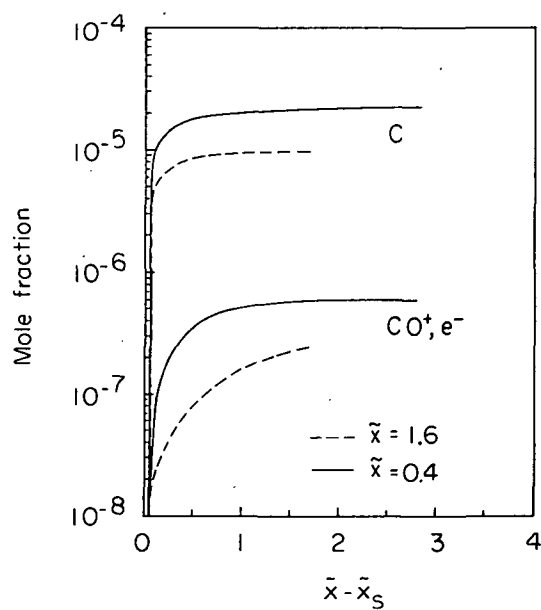


Figure 38.- Temperature variation along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6 . Case V.



(a) A, CO, O, and CO₂.



(b) C, CO⁺, and e⁻.

Figure 39.- Species concentrations along streamlines crossing the shock at $\tilde{x} = 0.4$ and 1.6 . Case V.

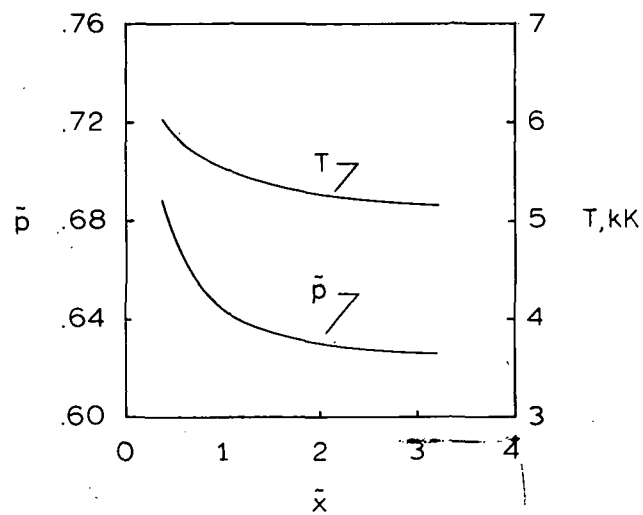
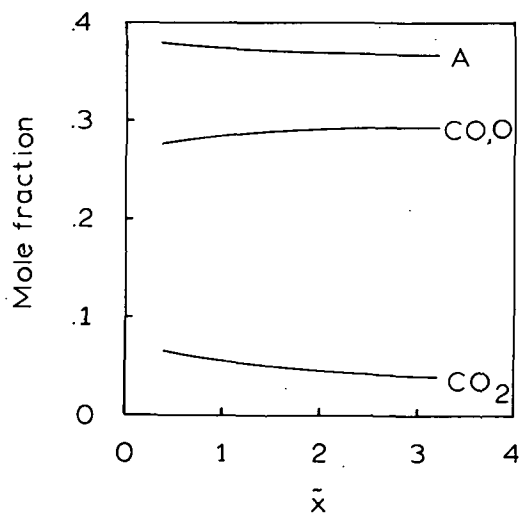
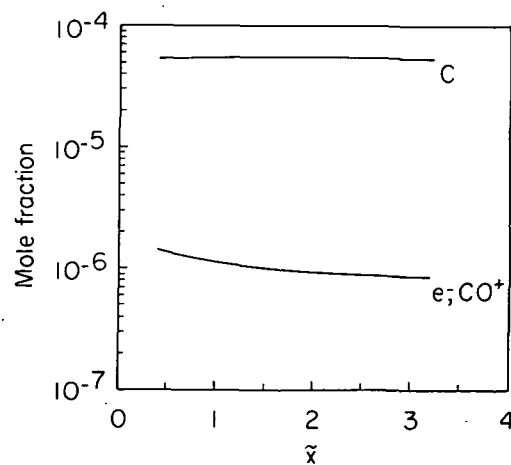


Figure 40.- Pressure and temperature variations along body surface. Case V.



(a) A, CO, O, and CO₂.



(b) C, CO⁺, and e⁻.

Figure 41.- Species concentrations along body surface. Case V.

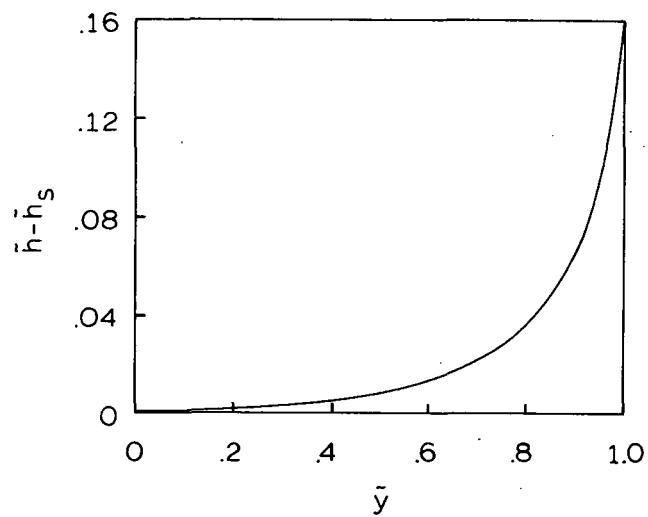


Figure 42.- Static enthalpy profile across shock layer at $\tilde{x} = 1.6$. Case V.

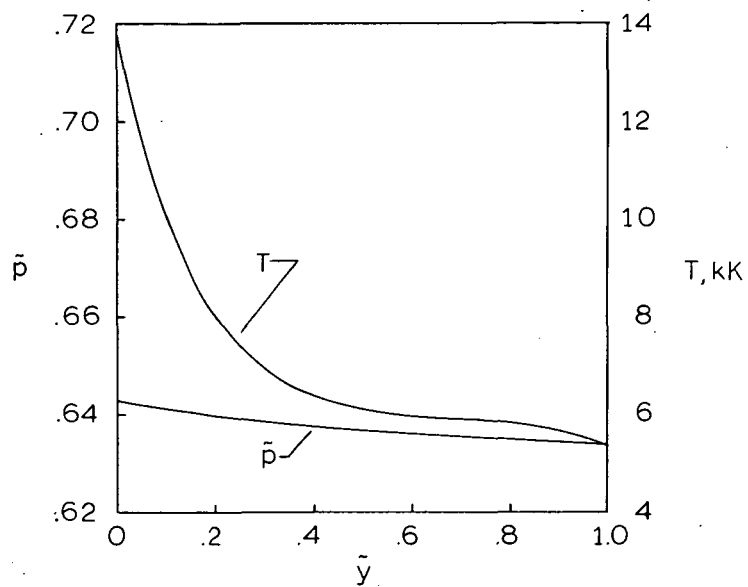


Figure 43.- Pressure and temperature profiles across the shock layer at $\tilde{x} = 1.6$. Case V.

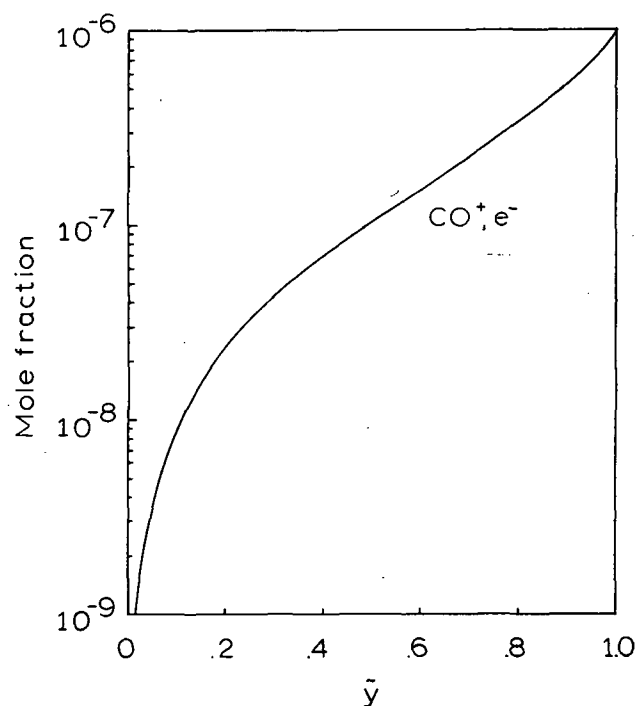


Figure 44.- Electron concentration profile across the shock layer at $\tilde{x} = 1.6$. Case V.

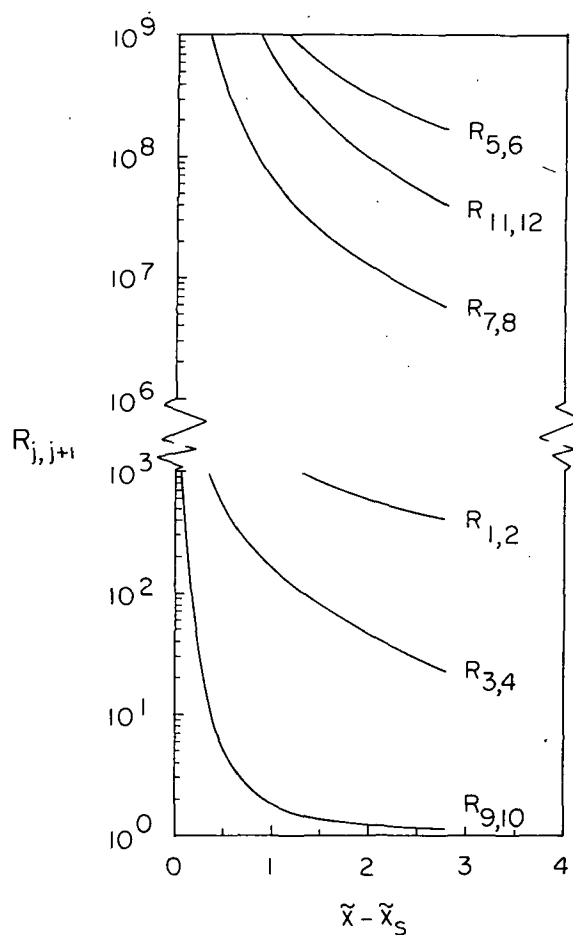


Figure 45.- Ratio of forward reaction rate to reverse reaction rate along inner streamline. ($\tilde{x} = 0.4$). Case V.

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— NATIONAL AERONAUTICS AND SPACE ACT OF 1958

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