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

by William L. Grose
Langley Research Center
Hampton, Va. 23365

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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 jth reaction

a  speed of sound, cm/sec

a_{i,j}  correlation integers for ith species in jth reaction (see appendix B)

B_j  temperature exponent in rate constant for jth reaction

c_i  mass fraction of ith species

E_j  activation energy in rate constant for jth reaction, K

e  internal energy per unit mass, ergs/g

e_{e,i}  electronic energy per unit mass of ith species, ergs/g

e_i  internal energy per unit mass of ith species, ergs/g

e_{v,i}  vibrational energy per unit mass of ith species, ergs/g

\bar{e}_{v,i}  equilibrium vibrational energy per unit mass of ith 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 lth electronic energy level of ith species

\Delta H_i  standard heat of formation at 0 K of ith species, ergs/mole

h  static enthalpy per unit mass, ergs/g

\tilde{h} = h/V_\infty^2

K_j  rate constant for jth reaction, (moles)^{1-n}(cm)^{3n-3}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

\( N_j \) number of vibrational energy levels included in dissociation energy of ith species

\( n \) order of reaction

\( p \) pressure, dynes/cm²

\( \bar{p} = \frac{p}{p_\infty} v_\infty^2 \)

\( q_k \) general parameter representing either vibrational energy per unit mass or mass fraction of kth species

\( R \) universal gas constant, \( 8.3147 \times 10^7 \) 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

\( \bar{r} = r/R_n \)

\( [S_i] \) moles per unit volume of ith species, moles/cm³

\( S_j \) \( S_j = 1 \) if \( \nu_{i_{+1},j} = 0 \); \( S_j = \frac{a_{i,j} C_1}{\mu_i} \) 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

$\Delta_i$  
  dissociation energy of $i$th species, K

$\delta$  
  function defined in equation (49)

$\epsilon_{i,l}$  
  energy of $l$th electronic level of $i$th species, K

$\Theta_i$  
  characteristic vibrational temperature, K

$\theta$  
  local shock inclination angle (see fig. 1)
A function defined in equation (47)

\( \Lambda \)

scale factor \((1 - y)/R_c\)

\( \lambda \)

molecular weight of gas mixture, g/mole

\( \mu \)

molecular weight of ith species, g/mole

\( \mu_i \)

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

\( \rho \)

mass density, g/cm³

\( \tilde{\rho} = \rho/\rho_\infty \)

\( \sigma_{i,k} \)

coefficient in vibrational relaxation time expression

\( \tau_{i,k} \)

vibrational relaxation time of ith species due to vibrational energy exchange with kth species, sec

\( \phi \)

angular position coordinate (fig. 1)

\( \phi_j \)

coupling factor defined in equation (40)

\( \psi \)

stream function, g/sec

\( \Omega \)

function defined in equation (48)

\( \omega_k \)

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
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:

\[
\frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) = 0
\]  

(1)

Momentum equations:

\[
\begin{align*}
\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} - \frac{\partial p}{\partial x} + \frac{1}{\rho} \frac{\partial \rho}{\partial x} &= 0 \\
\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \frac{u^2}{R_c} + \frac{\lambda}{\rho} \frac{\partial \rho}{\partial y} &= 0 
\end{align*}
\]  

(2)

(3)

Energy equation:

\[
\frac{h}{2} + \frac{u^2}{2} + \frac{v^2}{2} = \text{Constant}
\]  

(4)

Rate equation:

\[
\rho \frac{\partial q_k}{\partial x} + \lambda \rho \frac{\partial q_k}{\partial y} = \lambda \omega_k (\rho, p, q_1, \ldots, q_N)
\]  

(5)

Equation of state:

\[
h = h(p, \rho, q_1, \ldots, q_N)
\]  

(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,

\[
\frac{\partial \psi}{\partial x} = \rho v r \lambda
\]  

(7)
\[
\frac{\partial \psi}{\partial y} = -\rho ur
\]  

which leads to the transformation relationship
\[
\left( \frac{\partial}{\partial x} \right)_\psi = \frac{\partial}{\partial x} + \frac{\lambda v}{u} \frac{\partial}{\partial y}
\]  

The resulting expressions for the momentum and rate equations are
\[
\left( \frac{\partial u}{\partial x} \right)_\psi = \frac{v}{R_c} + \frac{\lambda vr}{u} \left( \frac{\partial p}{\partial \psi} \right)_x + \frac{1}{\rho u} \left( \frac{\partial p}{\partial x} \right)_\psi = 0
\]  

\[
\left( \frac{\partial v}{\partial x} \right)_\psi = \frac{u}{R_c} - \lambda r \left( \frac{\partial p}{\partial \psi} \right)_x = 0
\]  

\[
\left( \frac{\partial q_k}{\partial x} \right)_\psi = \frac{\lambda \omega_k}{u}
\]  

A differential form of the energy equation results from differentiating equation (4) and combining it with equations (2) and (3)
\[
\left( \frac{\partial h}{\partial x} \right)_\psi = \frac{1}{\rho} \left( \frac{\partial p}{\partial \psi} \right)_x
\]  

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
\[
\left( \frac{\partial p}{\partial \psi} \right)_x = \frac{u}{R_c r}
\]  

\[
\left( \frac{\partial q_k}{\partial x} \right)_\psi = \frac{\omega_k}{u}
\]  

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
\[
p(x, \psi) = p_s(x) + \frac{u_s(x)}{R_c(x) r_s(x)} \left[ \psi - \psi_s(x) \right]
\]
At the shock

$$\psi_s = \frac{\rho_{\infty} V_{\infty} r_s^2}{2}$$

and on the body the boundary condition is

$$\psi_b = 0$$

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,

$$h + \frac{u^2}{2} + \frac{v^2}{2} = h_0 + \frac{v_0^2}{2}$$

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

$$v^2 - v_0^2 \ll u^2$$

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

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

In summary, equations (6), (13), (15), (16), and (21) form a determinate system of equations that can be integrated stepwise along streamlines to yield \( p, \rho, h, u, \) 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

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

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

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

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

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

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

$$h = e + \frac{P}{\rho}$$  \hspace{1cm} (29)$$

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

$$h = h\left(p; \rho; e_{x,i}, \cdots, e_{y,i}; c_{i}, \cdots, c_{I}\right)$$  \hspace{1cm} (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 \(i = 1, 2, 3, \ldots, I\) and the associated kinetic reactions \(j = 1, 2, 3, \ldots, J\).

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

$$\sum_{i=1}^{I} \nu_{i}S_{i} \longrightarrow \sum_{i=1}^{I} \nu'_{i}S_{i}$$  \hspace{1cm} (31)$$

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

$$\frac{d}{dt} \left(\frac{[S_{i}]}{\rho}\right) = \frac{K}{\rho} \left(\nu'_{i} - \nu_{i}\right) \prod_{i=1}^{I} [S_{i}]^{\nu_{i}}$$  \hspace{1cm} (32)$$

Since

$$[S_{i}] = \frac{\rho c_{i}}{\mu_{i}}$$  \hspace{1cm} (33)$$

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

$$\left[\frac{\partial c_{i}}{\partial x}\right]_{j} = \frac{K_{j} \mu_{i}}{\rho u} \left(\nu'_{i,j} - \nu_{i,j}\right) \prod_{i=1}^{I} \left(\frac{\rho c_{i}}{\mu_{i}}\right)^{\nu_{i,j}}$$  \hspace{1cm} (34)$$

11
The total rate of production is

$$\left( \frac{\partial c_i}{\partial x} \right)_j = \sum_{j=1}^{I} \left[ \frac{\partial c_i}{\partial x_j} \right]_{j}$$

(35)

The specific reaction rate constant is given by

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

(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

$$\left[ \frac{\partial c_i}{\partial x} \right]_{j} = \frac{K_j \mu_i (\nu_{i,1} - \nu_{i,j})}{\rho \sum_{i=1}^{I} \left( \rho c_i \mu_i \right)^{\nu_{i,j}}} \left[ \rho \sum_{i=1}^{I} \frac{c_i a_{i,j}}{\mu_i} \right]^{\nu_{i,1,1,j}}$$

(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

$$\left( \frac{\partial^2 e_{v,i}}{\partial x} \right)_j = \frac{1}{u} \sum_{k=1}^{I} \frac{c_k}{\tau_{i,k}} (\bar{e}_{v,i} - e_{v,i})$$

(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

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

(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

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

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

\[ N_i > \frac{\Delta_i}{\Theta_i} \] (41)

Inserting the coupling coefficient in equation (37) results in

\[
\left[ \frac{\partial c_i}{\partial x} \right] = \left[ \frac{\phi_j K \mu_1}{\rho a} \left( \nu_{i,j} - \nu_{i,j} \right) \right] \left[ \frac{1}{I} \left( \frac{\rho c_i}{\mu_1} \right)^{\nu_{i,j}} \right] \left[ \rho \sum_{i=1}^{I} \frac{c_i a_{i,j}}{\mu_1} \right]^{\nu_{i+1,j}}
\]

(42)

For a dissociation reaction, \( \phi_j \) can be calculated from equation (40); for other reactions, \( \phi_j \) 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
\[ r_s = r_s(z) \] (43)

was used. From this relationship, \( \theta \), \( R_c \), and \( x \) can be given by

\[ \theta = \arctan \left( \frac{dr_s}{dz} \right) \] (44)

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

and

\[ x = \int_0^{r_s} \frac{dr_s}{\sin \theta} \] (46)

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

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:

\[ \Lambda(x) = p_\infty V_\infty \sin \theta \] (47)

\[ \Omega(x) = p_\infty + p_\infty V_\infty^2 \sin^2 \theta \] (48)

\[ \delta(x) = e_\infty + \frac{p_\infty}{\rho_\infty} + \frac{V_\infty^2 \sin^2 \theta}{2} \] (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
Equation (50) can be iterated until subsequent values of \( T_s \) differ by a sufficiently small amount. After convergence

\[
T_s = \frac{2\mu_\infty (\delta - e_s) \sqrt{\Omega^2 - 2\Lambda^2(\delta - e_s)}}{R \left[ \Omega + \sqrt{\Omega^2 - 2\Lambda^2(\delta - e_s)} \right]}
\]  (50)

The pressure distribution in the \( x, \psi \) 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 \( \psi \) 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 \( \Delta x \) 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 \( \psi \) 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 \(\psi\). 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 catar- nary shock \((R_{c,0} = 2.11 \text{ cm})\) with a free-stream velocity of \(7.01 \times 10^5 \text{ cm/sec at 61 km}\). 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 \(\theta\) of \(81^\circ\) \((x/R_{c,0} = 0.16)\). 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 θ = 81° 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

\[ r_s^2 = -0.3625z_s^2 + 36.064z_s - 0.1767r_sz_s \]  

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

\[ z_s = \frac{r_s^2}{1 + Ar_s} \]  

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.
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 $\text{CO}_2$ 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 $57^\circ$ half-angle sphere-cone are shown in figure 15. Pressure, density, and temperature variations along streamlines crossing the shock at $\bar{x} = 0.5$ 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 $\text{CO}_2$ disappears rapidly with increasing distance while the C and O concentrations increase along the inner streamline ($\bar{x} = 0.5$). The CO concentration increases to a maximum and then decreases. Figure 19(b) shows similar behavior along the outer streamline ($\bar{x} = 2.0$). This behavior is the same as that observed by Howe, Viegas, and Sheaffer (ref. 36) behind normal shocks in $\text{CO}_2$ 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 $\text{C}^+$ and $\text{O}^+$ ions increase with distance whereas $\text{CO}^+$ reaches a maximum and then begins to decrease along the inner streamline ($\bar{x} = 0.5$). The same behavior is exhibited along the outer streamline ($\bar{x} = 2.0$) except that the $\text{CO}^+$ 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\textsubscript{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 $\bar{x} = 2.0$. 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 $\bar{x} = 2.0$ 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\textsubscript{2} and 5 percent A by mass. The free-stream conditions are:

\begin{align*}
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}
\end{align*}

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

$$z_s = \frac{r_s^2}{1 + 1.89r_s}$$

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

Species concentrations along these same streamlines are presented in figure 29. The CO\textsubscript{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 \( \bar{x} = 1.6 \). Pressure and temperature profiles across the shock layer at this value of \( \bar{x} \) 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 \( \rho_{\infty} = 3.5 \times 10^{-7} \) g/cm³. 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

\[
R_j = \frac{K_j I}{\rho} \left( \frac{\rho c_{i,j}}{\mu_i} \right)^{\nu_{i,j} - 1} \rho \sum_{i=1}^{I} \frac{c_i a_{i,j}}{\mu_i}
\]

(58)

and define the ratio

\[
R_{j,j+1} = \frac{R_j}{R_{j+1}}
\]

(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 (\( \bar{x} = 0.4 \)) 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 furthermost 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 $\rho_\infty$ 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

$$z_s = \frac{r_s^2}{1 + 1.98r_s}$$

(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 programmed 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 programming 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,  
APPENDIX A

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

By Barbara L. Weigel
Langley Research Center

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 \((x_s, z_s, r_s, R_c, \cos \theta, \text{ and } \sin \theta)\) from a definition supplied by the user. (See fig. 1)

2. Computation of the free-stream quantities \(\left( \mu_\infty, \rho, a_\infty, M_\infty, \text{ and } e_\infty \right)\)

3. Computation of quantities immediately behind the shock \(\left( e_s, T_s, p_s, \rho_s, u_s, \text{ and } \psi_s \right)\)

4. Computation of pressures, and their derivatives, in the flow field \(\left( p(x, \psi) \text{ and } \frac{dp}{dx}(x, \psi) \right)\)

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 \(r, y, \text{ and } z\), at specified points in the flow field to give a good body and flow field definition
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:

<table>
<thead>
<tr>
<th>FORTRAN name</th>
<th>Called by</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>SHOCKG</td>
<td>D1290</td>
<td>to compute the shock geometry and store on tape 10</td>
</tr>
<tr>
<td>FDPDX</td>
<td>D1290</td>
<td>to evaluate the pressure p and its derivative ( \dot{p} ) and store on tapes</td>
</tr>
<tr>
<td>FOFTS</td>
<td>ITR1</td>
<td>to evaluate ( T_S )</td>
</tr>
<tr>
<td>ITR1</td>
<td>BASIC</td>
<td>to iterate for ( e )</td>
</tr>
<tr>
<td>ITR1</td>
<td>D1290</td>
<td>to iterate for ( T_S )</td>
</tr>
<tr>
<td>CALINTH</td>
<td>D1290</td>
<td>to obtain the integration technique</td>
</tr>
<tr>
<td>BASIC</td>
<td>CALINTH</td>
<td>to evaluate the derivatives ( \dot{h}, \dot{c}<em>i, \text{ and } \dot{e}</em>{v,i} ) for ( i = 1, I )</td>
</tr>
<tr>
<td>FOFE</td>
<td>ITR1</td>
<td>to evaluate ( e )</td>
</tr>
<tr>
<td>CHECK</td>
<td>CALINTH</td>
<td>to test results of an integration step and accept or reject the results</td>
</tr>
</tbody>
</table>
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, cos θ, and sin θ. These six parameters must be computed at each x from x = 0 to x ≤ ZSTERM and x must be in increments of DELX/5 to DELX and increments of DELX thereafter until x ≤ ZSTERM where

x  distance along shock, cm
z  distance along symmetry axis, cm
r  perpendicular distance from symmetry axis to shock, cm
R   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 \( h - 0.000001 \times h \) and one more iteration on \( e \) is attempted.
(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 \( T_{v,i} \) \((i = 1, I)\), \( u, \rho, p, \) and \( p \) values are computed and the \( \psi = 0.0 \) streamline is integrated from \( \Delta x \) to \( x \geq ZSTERM \).

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:

<table>
<thead>
<tr>
<th>FORTRAN name</th>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NAM1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DELX</td>
<td>( \Delta x )</td>
<td>increment along shock, cm</td>
</tr>
<tr>
<td>ZSTERM</td>
<td></td>
<td>length of symmetry axis, ( z, cm )</td>
</tr>
</tbody>
</table>
APPENDIX A – Continued

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

<table>
<thead>
<tr>
<th>FORTRAN name</th>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NULJ</td>
<td>$\nu_{i,j}$</td>
<td>a two-dimensional array of stoichiometric coefficients of $i$th reactant in $j$th reaction</td>
</tr>
<tr>
<td>NUPLJ</td>
<td>$\nu_{i,j}$</td>
<td>a two-dimensional array of stoichiometric coefficients for $i$th product in $j$th reaction</td>
</tr>
<tr>
<td>ALPIK</td>
<td>$\alpha_{i,k}$</td>
<td>a two-dimensional array of coefficients in vibrational relaxation time expression</td>
</tr>
<tr>
<td>BETAIK</td>
<td>$\beta_{i,k}$</td>
<td>a two-dimensional array of temperature exponents in vibrational relaxation time expression</td>
</tr>
<tr>
<td>SIGIK</td>
<td>$\sigma_{i,k}$</td>
<td>a two-dimensional array of coefficients in vibrational relaxation time expression</td>
</tr>
<tr>
<td>THETAI</td>
<td>$\Theta_i$</td>
<td>an array containing characteristic vibrational temperature $K$ for each species $i$</td>
</tr>
<tr>
<td>DGENI</td>
<td>$g_i$</td>
<td>an array of factors for each species $i$ to permit approximating a polyatomic molecule by a diatomic molecule</td>
</tr>
<tr>
<td>FI</td>
<td>$f_i$</td>
<td>an array of correlation factors for each species $i$, 0.0 for monatomic species and 1.0 for all others</td>
</tr>
<tr>
<td>DELHI</td>
<td>$\Delta H_i$</td>
<td>an array of standard heat of formation at 0 K for each species $i$, ergs/mole</td>
</tr>
<tr>
<td>DELI</td>
<td>$\Delta_i$</td>
<td>an array of dissociation energy for each species $i$, K</td>
</tr>
<tr>
<td>EVI</td>
<td>$e_{v,i}$</td>
<td>an array of vibrational energy per unit mass for each species $i$, ergs/g</td>
</tr>
<tr>
<td>FORTRAN name</td>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>LI</td>
<td>( \text{L}_i )</td>
<td>an array containing number of electronic levels for each species ( i )</td>
</tr>
<tr>
<td>GIL</td>
<td>( \varepsilon_{i,l} )</td>
<td>a two-dimensional array containing degeneracy of LI electronic levels for each species ( i )</td>
</tr>
<tr>
<td>EPSIIIL</td>
<td>( \varepsilon_{i,l} )</td>
<td>a two-dimensional array containing energy of LI electronic levels for each species ( i ), ( 0^\circ \text{K} )</td>
</tr>
<tr>
<td>AJ</td>
<td>( A_j )</td>
<td>an array containing frequency factor, ( \text{cm}^3\text{n}/\text{mole}^n\cdot\text{sec} ), for each reaction ( j ) in Arrhenius-type rate equation</td>
</tr>
<tr>
<td>XI</td>
<td></td>
<td>the initial computing interval. If no XI is input, 0.0001220703125 will be used</td>
</tr>
<tr>
<td>ELE1</td>
<td></td>
<td>an array of ( 2(\text{IMAX}) + 1 ) values used by integration scheme to control size of computing interval. ( 0.0 &lt; \text{ELE1} \leq 64.0 )</td>
</tr>
<tr>
<td>ELE2</td>
<td></td>
<td>an array of ( 2(\text{IMAX}) + 1 ) values used by integration scheme to control size of computing interval. ( \text{ELE2} &lt; \text{ELE1} )</td>
</tr>
<tr>
<td>XPST</td>
<td></td>
<td>an array of ( x ) values at which physical space calculations are desired. They must be multiples of ( \text{DELX} ). The program sets ( \text{XPST}(1) = \text{DELX} ) and ( \text{XPST}(\text{NXPST}) = [x \text{ at ZSTERM}] + 100.0 )</td>
</tr>
<tr>
<td>NXPST</td>
<td></td>
<td>number of values in XPST array ( \leq 100 )</td>
</tr>
<tr>
<td>IPF</td>
<td></td>
<td>PRINT ANSWERS every IPF integration; ( \text{IPF} = 5 ) unless input otherwise</td>
</tr>
</tbody>
</table>
### APPENDIX A – Continued

#### FORTRAN

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CIMAX</td>
<td></td>
<td>maximum computing interval; if CIMAX is not input, 0.0625 will be used</td>
</tr>
<tr>
<td>TIMER</td>
<td></td>
<td>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</td>
</tr>
<tr>
<td>IPICKUP</td>
<td></td>
<td>= 1 to pickup case from tape 13 = 0 unless input</td>
</tr>
<tr>
<td>IBUG</td>
<td></td>
<td>an array of 15 integers which must be input as 0 to trigger debug printouts at critical points (see Program Listing'</td>
</tr>
</tbody>
</table>

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
SNAM =
M = 0,
MUI(1) = 26.016, 32.000, 14.008, 16.000, 30.008, 30.008, 5.04862E-4,
CIINF(1) = 0.0768, 232.000, 0, 0, 0, 0, 0,
PINF = 1.98E2,
TINF = 253.8,
VINF = 7.02E5,
```
\[ R = 8.31469 \times 10^7 \]
\[ \Gamma = 1.4 \]
\[ \text{G}: (1) \]
\[ G(1) = 1.0 \times 10^6 + 0.2 + 0.4 \times 10^7 \]
\[ G(2) = 3.0 \times 10^5 + 0.3 + 0.3 \times 0.2 \]
\[ G(3) = 4 \times 10^5 + 4 \times 10^7 \]
\[ G(4) = 5 \times 10^5 + 1 \times 10^7 \]
\[ G(5) = 2 \times 10^4 + 2 \times 10^4 + 2 \times 10^4 \]
\[ G(6) = 1 \times 10^7 + 3 \times 10^7 \]
\[ G(7) = 1 \times 10^7 + 1 \times 10^7 \]
\[ D(1) = 20 \times 10^7 \]
\[ \text{E}: (1) \]
\[ E(1) = 0.7 \times 10^5 \]
\[ E(2) = 0.1 \times 10^5 \]
\[ E(3) = 0.3 \times 10^5 \]
\[ E(4) = 0.5 \times 10^5 \]
\[ E(5) = 0.7 \times 10^5 \]
\[ E(6) = 0.9 \times 10^5 \]
\[ E(7) = 1 \times 10^7 \]
\[ E(8) = 1.2 \times 10^7 \]
\[ E(9) = 1.4 \times 10^7 \]
\[ E(10) = 1.6 \times 10^7 \]
\[ E(11) = 1.8 \times 10^7 \]
\[ E(12) = 2 \times 10^7 \]
\[ E(13) = 3 \times 10^7 \]
\[ E(14) = 4 \times 10^7 \]
\[ E(15) = 5 \times 10^7 \]
\[ E(16) = 6 \times 10^7 \]
\[ E(17) = 7 \times 10^7 \]
\[ E(18) = 8 \times 10^7 \]
\[ E(19) = 9 \times 10^7 \]
\[ E(20) = 1 \times 10^8 \]
APPENDIX A – Continued

AI(1+11) = 7*0.
AI(1+12) = 7*0.
AIPIK(1+1) = 7*5.675E-4,
AIPIK(1+2) = 7*1.443E-7.
AIPIK(1+3) = 7*0.
AIPIK(1+4) = 7*0.
AIPIK(1+5) = 7*1.513E-4,
AIPIK(1+6) = 7*1.513E-4.
BETAIK(1+1) = 7*0.09952,
BETAIK(1+2) = 7*0.37177,
BETAIK(1+3) = 7*0.
BETAIK(1+4) = 7*0.
BETAIK(1+5) = 7*0.2226.
BETAIK(1+6) = 7*0.2226.
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.
ELE(1) = 42#64.
ELE(2) = 42#1.0.
XI = 0.0625,
ZTERM = 1.145,
DELX = 0.06,
TCHEKT = 0.3,
HCHEKT = 0.01,
PHMAX = 65.0.
EV1(1) = 20*0.0.
NXPST = 15.
XPST(1) = 0.06, 0.12, 0.18, 0.24, 0.3, 0.36, 0.42, 0.48, 0.54, 0.6, 0.66, 0.72, 0.78, 0.84, 0.10.
IPF = 5,
TIMER = 240.0,
IPICKUP = 0.

N2 = 02 = 0
N2 + O = 02 + M
20 + M = 02 + M
N0 + M = N + O + M
N + O + M = NO + M
N0 + M = NO + M
N0 + N = N0 + 0
NO + N = NO + 0
N0 + O = N + O2
N + O = NO + E-
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 \( \psi \)
Tape 9, to save pressure at each x for each \( \psi \)
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 \( T_s, e_s, p_s, \rho_s, u_s, \psi_s, h_s, (e_v,i)_s \) (i = 1,IMAX) at each x
Tape 12, to save physical space data
Tape 13, pickup tape
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 110 000. The sample case was completed in two passes on the Control Data 6600 computer to illustrate the pickup capability.

Programmed 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
34
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 $\mu_\infty$, $\rho_\infty$, $a_\infty$, $M_\infty$, $e_{1,\infty}$, $e_{\infty}$, $(e_{e,i})_{\infty}$, and $(e_{v,i})_{\infty}$ ($i = 1, IMAX$)

7 the quantities behind the shock $T_s$, $e_s$, $p_s$, $\rho_s$, $u_s$, $\psi_s$, $h_s$, and $(e_{v,i})_s$ ($i = 1, IMAX$) for each streamline $\psi$ 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 $\psi$ at $x = DELX/5$

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

  $x,h,\mu,p$\bigg)_{\rho,u,T,e}$ for computing interval $\sum_{i=1}^{IMAX} c_i$

  $c_i$ ($i=1, IMAX$) concentration

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

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

  (IPSI=6) is used for the stagnation streamline, $\psi = 0.0$, and the streamline beginning at $\Delta x$

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
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.

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:
### APPENDIX A - Continued

#### SPECIES

1. N2
2. O2
3. N
4. O
5. NO
6. NO+
7. E-

#### REACTIONS

1. O2 + M = 2O + M
2. 2O + M = O2 + M
3. NO + M = N + O + M
4. N + C + M = NO + M
5. N2 + M = 2N + M
6. 2N + M = N2 + M
7. N + O2 = NO + O
8. NC + O = N + O2
9. N2 + O = NO + N
10. NO + N = N2 + O
11. NO+ + E- = N + O
12. N + O = NO+ + E-

#### PRINT FREQUENCY = 5

McCHECK = 1.000000000E+00  TCHECK = 3.660000000E-01  PMAX = 6.500000000E+01

XI = 6.250000000E-02  CMAX = 5.000000000E-01

ELE1 = 6.400000000E+01  6.400000000E+01


ELE2 = 1.000000000E+00  1.000000000E+00

1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00

1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00

1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00

1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00  1.000000000E+00

0.  0.  0.  0.  0.  0.  0.  0.  0.

NXPS = 15

XPSS =

6.100000000E+00  1.200000000E+01  1.800000000E+01  2.400000000E+01  3.000000000E+01  3.600000000E+01  4.200000000E+01

4.800000000E+01  5.400000000E+01  6.000000000E+01  6.600000000E+01  7.200000000E+01  7.800000000E+01  8.400000000E+01
<table>
<thead>
<tr>
<th>JU</th>
<th>THETA1</th>
<th>EGEN1</th>
<th>FI</th>
<th>DELHI</th>
<th>DEL1</th>
<th>CIINF</th>
<th>EVI</th>
<th>LI</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.20000000E+01</td>
<td>1.50000000E+00</td>
<td>5.49380000E+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.00000000E+18</td>
<td>-1.00000000E+00</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>5.20000000E+21</td>
<td>-1.50000000E+00</td>
<td>7.54900000E+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.30000000E+21</td>
<td>-1.50000000E+00</td>
<td>0.</td>
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<tr>
<td>1</td>
<td>3.00000000E+21</td>
<td>-1.50000000E+00</td>
<td>1.13260000E+05</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1</td>
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<td>-1.50000000E+00</td>
<td>0.</td>
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<td></td>
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</tr>
<tr>
<td>2</td>
<td>1.00000000E+12</td>
<td>5.00000000E-01</td>
<td>3.12000000E+03</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2.38000000E+11</td>
<td>5.00000000E-01</td>
<td>1.91300000E+04</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>5.00000000E+13</td>
<td>0.</td>
<td>3.80900000E+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>5</td>
<td>1.11000000E+13</td>
<td>0.</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1.80000000E+21</td>
<td>-1.50000000E+00</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.17000000E+11</td>
<td>1.20000000E-01</td>
<td>3.18580000E+04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>i=</td>
<td>1 (GILL(l),l=1,IMAX+1)</td>
<td>1.00000000E+00</td>
<td>3.00000000E+00</td>
<td>6.00000000E+00</td>
<td>2.00000000E+00</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>-----</td>
<td>-----------------------------------------</td>
<td>-----------------</td>
<td>----------------</td>
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<td>----------------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>0.</td>
<td>1 (EPEL(l,l),l=1,IMAX+1)</td>
<td>7.15920000E+04</td>
<td>8.53930000E+04</td>
<td>9.92120000E+04</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
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<tr>
<td>0.</td>
<td>1 (AIJ(l,l),l=1,IMAX)</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>1 (ALPIK(l,k,k=1,IMAX)</td>
<td>5.67500000E-04</td>
<td>5.67500000E-04</td>
<td>5.67500000E-04</td>
<td>5.67500000E-04</td>
<td>5.67500000E-04</td>
<td>5.67500000E-04</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>1 (BETAi(l,k,k=1,IMAX)</td>
<td>-9.95200000E-02</td>
<td>-9.95200000E-02</td>
<td>-9.95200000E-02</td>
<td>-9.95200000E-02</td>
<td>-9.95200000E-02</td>
<td>-9.95200000E-02</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>1 (SIGI(l,k,k=1,IMAX)</td>
<td>1.63630000E+02</td>
<td>1.63630000E+02</td>
<td>1.63630000E+02</td>
<td>1.63630000E+02</td>
<td>1.63630000E+02</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
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<td>1 (NUI(J,J),J=1,IMAX)</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>1.00000000E+00</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>1 (NUPI(J,J),J=1,IMAX)</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>1.00000000E+00</td>
<td>0.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>i=</th>
<th>2 (GILL(l),l=1,IMAX+1)</th>
<th>1.00000000E+00</th>
<th>3.00000000E+00</th>
<th>1.00000000E+00</th>
<th>3.00000000E+00</th>
<th>0.</th>
<th>0.</th>
<th>0.</th>
<th>0.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.</td>
<td>2 (EPEL(l,l),l=1,IMAX+1)</td>
<td>1.13420000E+01</td>
<td>1.88790000E+04</td>
<td>5.13650000E+04</td>
<td>5.21040000E+04</td>
<td>7.10260000E+04</td>
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<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>2 (AIJ(l,l),l=1,IMAX)</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>1.00000000E+00</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>0.</td>
<td>2 (ALPIK(l,k,k=1,IMAX)</td>
<td>1.44300000E-07</td>
<td>1.44300000E-07</td>
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## APPENDIX A – Continued

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**APPENDIX A – Continued**
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CII = 7.908462701E-01
CII = 0.
CII = 4.73899672D+10
CII = 0.

EVI = 0.

EVI = 4.42067044D+10

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2

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X = 3.1531250000-02
Y = 5.29868106E+03
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CII = 1.21094389D-01
CII = 1.11267565E-01
CII = 8.37371279E-04
CII = 2.62560755D+10
CII = 2.43077184D+10

EVI = 0.

EVI = 2.44774826D+10

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2

11

X = 6.27812530D-02
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CHECK: 3.08462353E+01

CHECK: 2.91829299E+01

CHECK: 3.08462353E+01

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--- CHECK = 6.02130000E+01  

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APPENDIX A - Continued
### APPENDIX A - Continued

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MU = 2.1642572E+01
P = 1.04795836E+05
RHO = 2.45028E+03
U = 1.34073262E-05
CIF = 6.2970000E-02
SUM(CIF) = 1.71171717E+05

CIF (1) = 6.01057540E-01
CIF (2) = 4.0533221E-03
CIF (3) = 4.31222966E-01
CIF (4) = 2.60855950E-01
CIF (5) = 4.7957321E-02

CIF (6) = 6.24187013D-04
CIF (7) = 1.41116728D-03
CIF (8) = 1.53918699D-01
CIF (9) = 2.64634562D-01
CIF (10) = 3.5454114E-02

CM (1) = 4.64671915E-06
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CM (3) = 2.1103498E-01
CM (4) = 2.7632777E-01
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CM (9) = 0.0
CM (10) = 2.7235022D+10

EV1 (1) = 2.82577262E+10
EV1 (2) = 2.66772595E+10
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U = 1.4726742E-05
CIF (1) = 6.2950000E-02
SUM(CIF) = 1.0138980E+00
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CIF (3) = 1.53918699E-01
CIF (4) = 2.64634562E-01
CIF (5) = 4.52479440E-02
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CIF (7) = 1.37866494E-03
CIF (8) = 0.0
CIF (9) = 0.0
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CM (5) = 3.2359482E-02
CM (6) = 5.38336461E-04
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CM (9) = 0.0
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EV1 (1) = 2.71568920E+10
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EV1 (4) = 0.0
EV1 (5) = 2.61725525E+00
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APPENDIX A - Continued

BEGIN PHYSICAL SPACE CALCULATIONS KSTAG = 119

\[ x = 6.00000000E-02 \]
\[ y = 5.40347303E-02 \]
\[ z = 2.10266976E-01 \]
\[ x = 5.99692100E-02 \]
\[ y = 2.69377752E-01 \]
\[ z = 9.07128054E-04 \]

\[ x = 1.20000000E-01 \]
\[ y = 1.11447842E-01 \]
\[ z = 1.57872841E-01 \]
\[ x = 1.20000000E-01 \]
\[ y = 1.14179895E-01 \]
\[ z = 1.04592015E-01 \]

\[ x = 1.20000000E-01 \]
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\[ z = 3.74030880E-03 \]

\[ x = 1.80000000E-01 \]
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\[ z = 1.36214231E-01 \]

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\[ z = 3.30704081E-02 \]

\[ x = 1.80000000E-01 \]
\[ y = 1.77141886E-01 \]
\[ z = 3.06679722E-03 \]
APPENDIX A – Continued
APPENDIX A - Continued

\[
\begin{array}{cccc}
\text{x}= 6.00000000E-01 & \text{R}= 5.57248692E-01 & \text{y}= 1.2701203E+01 & \text{z}= 2.06759283E-01 & \text{PSI}= 5.44413800E-03 \\
\text{x}= 6.00000000E-01 & \text{R}= 5.1755717E-01 & \text{y}= 1.10531504E-01 & \text{z}= 1.90940276E-01 & \text{PSI}= 8.8813814E-02 \\
\text{x}= 6.00000000E-01 & \text{R}= 5.66849084E-01 & \text{y}= 9.1830028E-02 & \text{z}= 1.72984081E-01 & \text{PSI}= 2.13146707E-02 \\
\text{x}= 5.00000000E-01 & \text{R}= 5.7246801E-01 & \text{y}= 7.13632015E-02 & \text{z}= 1.53245745E-01 & \text{PSI}= 1.64400873E-02 \\
\text{x}= 5.00000000E-01 & \text{R}= 5.78565507E-01 & \text{y}= 4.90233357E-02 & \text{z}= 1.31766562E-02 & \text{PSI}= 2.14070611E-02 \\
\text{x}= 5.00000000E-01 & \text{R}= 5.8513275E-01 & \text{y}= 4.913973E-02 & \text{z}= 1.05493157E-02 & \text{PSI}= 3.32936805E-02 \\
\text{x}= 6.00000000E-01 & \text{R}= 5.91970299E-01 & \text{y}= -1.9135480E-01 & \text{z}= 8.46143101E-02 & \text{PSI}= 3.32936805E-02 \\
\end{array}
\]
APPENDIX A – Continued

Complete Program

The complete program including comments for the sample case, the flow diagram, and the deck setup is reproduced herein.

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

C
C TAPE8 TO SAVE DERIVATIVE OF PRESSURE AT EACH X FOR EACH PSI
C TAPE9 TO SAVE PRESSURE AT EACH X FOR EACH PSI
C TAPE10 TO SAVE X AND CORRESPONDING ZS, RS, RC, COST, SINT
C TAPE11 TO SAVE TS, ES, PS, RHOS, US, PSIS, HS, (EVIS(I), I=1, IMAX)
C TAPE12 TO SAVE PHYSICAL SPACE DATA
C TAPE13 TO SAVE COMMON FOR PICKUP TAPE

C BL WEIGEL FOR WILLIAM L GROSE, APD, GAS PHYSICS SECTION
C INVERSE TECHNIQUE FOR DETERMINING THE FLOW FIELD IN A SHOCK
C LAYER ABOUT A SMOOTH SYMMETRIC BODY TRAVELING AT HYPERSONIC
C SPEEDS
C PHASE 3, A DIRECT NON-EQUILIBRIUM CALCULATION
C
C CALINTH, INTEGRATION ROUTINE
C THE NUMERICAL INTEGRATION ALGORITHM USED IS FOUND IN -A METHOD
C FOR THE NUMERICAL INTEGRATION OF COUPLED FIRST ORDER
C DIFFERENTIAL EQUATIONS WITH GREATLY DIFFERENT TIME CONSTANTS-
C BY CHARLES E. TREANOR, CONTRACT NO. NASR-119, CAL REPORT NO.
C AG-1729-A-4, JANUARY 1964, CORNELL AERONAUTICAL LABORATORY, INC.
C CORNELL UNIVERSITY, BUFFALO, N.Y.
C
C ITR1 - NEWTON-RAPHSON ITERATION METHOD
C FTLUP - INTERPOLATION ROUTINE

R     *SHOCK
1     *
1     *
1     *
1     *
1     *
1     *
1     *
1
1

C B SHOCK GEOMETRY

C

INPUT
C READ IN I CARD, 80 COLUMNS, BY FORMAT(3A10) FOR CASE ID
C INPUT DEFINITIONS --- NAMELIST INPUT

$NAM1
C DELX = INCREMENT ALONG SHOCK
C ZTERM= LENGTH OF SYMMETRY AXIS, Z
C IMAX = MAXIMUM NUMBER OF I-S, SPECIES, LESS THAN OR = 25
C JMAX = MAXIMUM NUMBER OF J-S, REACTIONS, LESS THAN OR = 50
C IBUG = 0 DEBUG PRINT OUTS
C = 1, NO DEBUG PRINT OUTS, 1 UNLESS INPUT OTHERWISE
C MJ = CODE INDICATING WHICH SPECIES, I, TO USE TO CALCULATE
C COUPLING FACTOR, PHI SUB J, FOR REACTION J
C R = UNIVERSAL GAS CONSTANT, ERG/MOLE DEG K
C GAMMA = RATIO OF SPECIFIC HEATS
C CIINF = FREE STREAM MASS FRACTION FOR EACH SPECIES
```

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APPENDIX A – Continued

PINF = FREE STREAM PRESSURE, DYNES/CM**2
TINF = FREE STREAM TEMPERATURE, DEG.K
VINF = FREE STREAM VELOCITY, CM/SEC
MUI = MOLECULAR WEIGHT FOR EACH SPECIES, GM/MOLE
THETAI = CHARACTERISTIC VIBRATIONAL TEMPERATURE, DEG.K
OGENI = FUDGE FACTOR TO PERMIT APPROXIMATING POLYATOMIC MOLECULE
BY DIATOMIC MOLECULE
FI = 0 FOR MONATOMIC SPECIES
= 1 FOR ALL OTHERS
DELHI = HEAT OF FORMATION, ERGS/MOLE
DELI = DISSOCIATION ENERGY OF SPECIES
EVI = VIBRATIONAL ENERGY OF SPECIES
LI = NUMBER OF ELECTRONIC LEVELS FOR EACH SPECIES, LI <= 20
EPSIL = L-TH ELECTRONIC ENERGY LEVEL FOR I-TH SPECIES
AJ = FREQUENCY FACTOR IN ARRHENIUS TYPE RATE EQ.
BJ = TEMPERATURE EXPONENT IN ARRHENIUS TYPE RATE EQ.
AIJ = FACTOR TO ALLOW USE OF GENERAL SPECIES IN REACTION EQUATIONS IF
DESIRED, = 1.0 OR = 0.0
NUIJ = STOICHIOMETRIC COEFFICIENTS OF I-TH REACTANT IN J-TH
REACTION
NUPIJ = STOICHIOMETRIC COEFFICIENT FOR I-TH PRODUCT IN J-TH
REACTION
ALPIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
BETAIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
SIGAIK = FACTORS IN EQ. FOR VIBRATIONAL RELAXATION TIME
XI = INITIAL COMPUTING INTERVAL, <= 0.001220703125 UNLESS INPUT.
ELE1 = (2*IMAX+1) VALUES USED BY INTEGRATION SCHEME
NORMALLY .1,.5 OR .05
ELE2 = (2*IMAX+1) VALUES USED BY INTEGRATION SCHEME
NORMALLY .05,.1 OR .01 AND LT ELE1
XPST = 99 OR LESS X-S AT WHICH PHYSICAL SPACE CALCULATIONS ARE
DESIRED. THEY MUST BE MULTIPLES OF DELX IN ORDER TO
HAVE RS,COST,IS AND SINT VALUES
AND LAST MUST BE = 0.0AT ZTERM.
THEREFORE, XPST(NXPST) SET = X AT ZTERM + 100.0 IN
PROGRAM
XPST(1) MAY NOT BE 0.0
THEREFORE, XPST(1) SET = DELX IN PROGRAM
NXPST = NUMBER OF X-S AT WHICH PHYSICAL SPACE CALCULATIONS ARE
DESIRED
IPF = PRINT FREQUENCY, 3 UNLESS INPUT OTHERWISE
IPF NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP RUNS
CIMAX = MAXIMUM CJ OR COMPUTING INTERVAL
0.0625 UNLESS INPUT OTHERWISE
CIMAX NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP RUNS
TIMER = TIME IN DECIMAL SECONDS, REQUESTED ON JOB CARD
IF THE JOB DOES NOT TERMINATE IN THE TIME ESTIMATED ON
THE JOB CARD, DATA FOR PICKUP WILL BE STORED ON TAPE 13.
IT IS = 3600.0 OR 1 HOUR UNLESS INPUT OTHERWISE
TIMER NOT IN COMMON THEREFORE IT MAY BE VARIED ON PICKUP RUNS
IPICKUP = 0 UNLESS INPUT
= 1 TO PICKUP CASE FROM TAPE 13
HCHECKT = CONTROL ON SIZE OF COMPUTING INTERVAL IN CHECK
IF(ABS(HPREV-H) = H*GT=HCHECK) REDUCE INTERVAL
TCHECKT = CONTROL ON SIZE OF COMPUTING INTERVAL IN CHECK
IF(ABS(TPREV-T) = T*GE=TCHECK) REDUCE INTERVAL
PHMAX = CONTROL ON COMPUTING INTERVAL, = 0.65.0

AFTER READING IN NAME, READ IN THE IMAX SPECIES BY FORMAT (8A10)
10 SPACES PER SPECIES
THEN READ IN THE JMAX REACTIONS BY THE SAME FORMAT USING 20
APPENDIX A — Continued

<table>
<thead>
<tr>
<th>C</th>
<th>SPACES PER REACTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>IF THE SPECIES AND REACTIONS ARE NOT READ IN,</td>
</tr>
<tr>
<td>C</td>
<td>IMAX/9 PLUS JMAX/4 BLANK CARDS MUST BE PUT IN THE DECK</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C</th>
<th>STOPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>STOP 1 INCORRECT INPUT</td>
</tr>
<tr>
<td>C</td>
<td>STOP 5 EOF 10 IN MAIN</td>
</tr>
<tr>
<td>C</td>
<td>STOP 13 IN SHOCKG</td>
</tr>
<tr>
<td>C</td>
<td>STOP 30 IN CHECK WHEN COMPUTING INTERVAL.LT.1.E-15</td>
</tr>
<tr>
<td>C</td>
<td>STOP 50 EOF 9 IN FDPDX</td>
</tr>
<tr>
<td>C</td>
<td>STOP 66 IN BASIC WHEN NO CONVERGENCE ON E ITERATION</td>
</tr>
<tr>
<td>C</td>
<td>STOP 301 IN MAIN FOR ERROR IN XPST ARRAY OR IZTERM.GT.500</td>
</tr>
<tr>
<td>C</td>
<td>STOP 321 ITRI STOP IN MAIN</td>
</tr>
<tr>
<td>C</td>
<td>STOP 422 IN MAIN AFTER PICKUP TAPE WRITTEN</td>
</tr>
<tr>
<td>C</td>
<td>STOP 563 IN MAIN WHEN XNE=VARI(IPS1)</td>
</tr>
<tr>
<td>C</td>
<td>STOP 665 IN MAIN AFTER AN INTEGRATION ATTEMPT</td>
</tr>
<tr>
<td>C</td>
<td>STOP 670 IN MAIN WHEN A CI NEGATIVE</td>
</tr>
</tbody>
</table>

| C | COMMON M,IX,IMAX,IPS1,IBUG(15) |
| C | COMMON P(500),OPDX(500),VARI(500) |
| C | FOLLOWING 7 VARIABLES DIMENSIONED BY IMAX |
| C | COMMON EVIINF(25),THETA(25),MUI(25),FI(25),DELI(25),CIINF(25),LI(25) |
| C | COMMON R,MUNINF,DELTA,OMEGA,LASSQ,OMEGAS,O,MO,T,U |
| C | FOLLOWING 2 VARIABLES DIMENSIONED BY (IMAX IN L1,IMAX) |
| C | COMMON EPSIIL(20,25),G1L(20,25) |
| C | COMMON VAR(52),CUVAR(52),DERI(51) |

| C | COMMON ZS,PS,RC,SINT,COST,PS,US,PSIS |
| C | FOLLOWING 4 VARIABLES DIMENSIONED BY JMAX |
| C | COMMON MUI(50),EJ(50),AJ(50),BJ(50) |
| C | FOLLOWING 3 VARIABLES DIMENSIONED BY IMAX |
| C | COMMON TII(25),NI(25),DGENI(25) |
| C | FOLLOWING 3 VARIABLES DIMENSIONED BY (IMAX+1,JMAX) OR (IMAX,JMAX) |
| C | COMMON NUIJ(25,50),AIJ(25,50),NUPIJ(25,50) |
| C | FOLLOWING 3 VARIABLES DIMENSIONED BY (IMAX,IMAX) |
| C | COMMON SIGIM(25,25),ALPIK(25,25),BETAIK(25,25) |
| C | COMMON KSTAG,IMAXP2,IMAXL,N,IG,ISTAG,LS1,LS2,LS1,IMAXP1 |
| C | COMMON X,TS,ES,RHOS,HS,RHOUR,PHMAX,AAAAA,PREPSIS,PREX,PREU |
| C | COMMON EVISJIMAX) |
| C | COMMON EVIS(25),XPST(100) |

| C | COMMON /LAB2/ DELX,ZSTERM,IZTERM |
| C | COMMON /LAB3/ EINF,PINF,RHINF,VINF,E,JMAX,KEYINT,RHO,HSTAG |

| C | COMMON /LAB4/ PFTL,KI11,ETRI |
| C | COMMON /LAB5/ JUNEQ |
| C | COMMON /LAB6/ ELB,SPEC,CJ,TPREV,HPREV,HCHECK,TCHECK |
| C | COMMON /LAB7/ ITNEG,EEXP |
| C | COMMON /LAB8/ ELE1(51),ELE2(51),NERR |
| C | SPECIE(IIMAX),REACT(JMAX),DELI(IMAX) |
| C | DIMENSION SPECIE(25),REACT(50),IN(8),DELI(25) |

| C | DOUBLE PRECISION VAR,XVAR,H,CT,EVI |

| C | DIMENSION RUT(200),PSISTG(200) |
| C | DIMENSION ENG(11),ENGI(11) |
| C | DIMENSION CIG(25,6),EIG(25,6) |
| C | DIMENSION PSIG(5),TG(5),HG(6),CIT(6),EIT(6),EG(5) |
| C | DIMENSION CM(25),CII(25),EVI(25) |
| C | DIMENSION XX(3),XX(31) |

| C | XX AND XXX ARE TONK DIMENSIONS WHICH WILL CHANGE AS THE |
| C | DIMENSION STATEMENTS ARE CHANGED...THEY ARE USED FOR PICKUP RUN |
APPENDIX A – Continued

EQUIVALENCE (VAR(1), XVAR), (VAR(2), H), (VAR(3), CI(1))
EQUIVALENCE (VAR(2+IMAX+1), EVI(1))

REAL MUI, LAMSO, MUINF, MU
REAL NI
REAL MINF, MINFSO, LAMBDA
REAL NUIJ, NUPIJ

INPUT

NAME LIST/NAM1/ DELX, ZSTERM, 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, BETAIK, SIGIK, XI, CIMAX,
3 ELE1, ELE2, XPS, NXPST, IPF, TIMER, IPICKUP, HCHECK, TCHECK, PHMAX

EXTERNAL FOFTS

INITIALIZE

REWIND 8
REWIND 9
REWIND 10
REWIND 11
REWIND 12
REWIND 13
NERR=0

TIMER=3600.0
DO 5 I=1,15
IBUG(I)=1
NXPST=2
IPICKUP=0
ICHEK=0
ITNEG=0
IXP=0
NEG=0
IKG=0
IUNEG=0
DELZ=.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
READ INPUT
READ (5,15) (IN(I), I=1,8)
FORMAT (8A10)
READ (5, Nam1)
IF (IPICKUP.EQ.0) GO TO 60
PRINT 15, (IN(I), I=1,8)
READ PICKUP FROM TAPE13

THIS SHOULD PICKUP ALL COMMON AND LABLED COMMON
PLEASE CHECK DIMENSIONS IF THERE ARE PICKUP PROBLEMS

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 RECOUT (10, I=0, X, ZS, RS, RC, COST, SINT)
READ (13) (DPDX(J), J=1, IZTERM)
APPENDIX A – Continued

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)
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
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 (24HJ PICKUP CASE ------)
PRINT 50, IMOAXL,(XPST(I),I=1,10),(ELE2(I),I=1,5)
50 FORMAT (1X,6HIMAXL=,13,/,X,5HXPST=,5E17.8/1X,5HELE2=,5E17.8/1X,1,6HKSTAG=,13/1)
PRINT 600, IPSI,I,IX,XVAR,H,MU,PFTL,RH0,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,IMAX)
SPEC=0
IX=IX-1
IBUG(11)=0
KEYINT=0
KIPF=IPF-1
HCHECK=HCHECKT
TCHECK=TCHECKT
PRINT 55, IPF,CIMAX,TIMER,HCHECK,TCHECK,IZTERM,KSTAG
55 FORMAT (1CH IPF = I2,10H CIMAX=E15.8,10H TIMER = E15.8,10H HCHECK = E15.8,10H TCHECK = E15.8,10H IZTERM = I2,10H KSTAG = I2/1)
GO TO 560
60 CONTINUE
C IF (IBUG(11).EQ.1) GO TO 65
WRITE (6,NAM1)
65 PRINT 70
70 FORMAT (1H1)
PRINT 15, (IN(I),I=1,8)
C SUM OF CIINF SHOULD BE 1.0
SUM=0.
DO 75 I=1,IMAX
  SUM=SUM+CIINF(I)
  IF (SUM.EQ.1.0) GO TO 85
  PRINT 80, SUM, (CIINF(I), I=1,IMAX)
  FORMAT (34H SUM OF CIINF SHOULD BE 1.0. IT IS,E17.8,8H CIINF=E5(5
1E17.8))
  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
  DO 110 I=1,JMAX
  105 FORMAT (ISPECIE(I))
  PRINT 95 ' - -'
  JMAX2=2*JMAX
  READ (15,90) (REACT!(I), I=1,JMAX2)
  PRINT 115
  115 FORMAT (14H REACTIONS/)
  J=0
  DO 120 I=1,JMAX2,2
  120 PRINT 125, J,REACT(J), REACT(J+1)
  125 FORMAT (I5,2A10)
  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=1,4XPSTP1)
  140 FORMAT (4H XI=E15.8/7H CIMAX=E15.8/6H ELE1=2E17.8/7(0E17.8)/6H EL
1E2=2E17.8/7(T/E17.8'/7H XPST=13/6H XPST=15(T/E17.8'/7/)
  PRINT 145, DELX,ZSTEM,TIMER,IPICKUP
  145 FORMAT (6H DELX=E15.8/8H ZSTEM=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=12,8H JMAX=12,5H M=1/3H R=E15.8/7H GAMMA=E15
18/6H PINF=E15.8/6H TINF=E15.8/6H VINF=E15.8/6H IBUG=I1,14I5/7)
  PRINT 155
  155 FORMAT (5X,3HMUI12X,6HTHETAI9X,5HGENI10X,2HFI13X,5HDELHI10X,4HDEL
1111X,5HCINF10X,3HEVI12X,2HLI//)
  DO 165 I=1,IMAX
  165 PRINT 160, MUI(I),THETAI(I),DGENI(I),FI(I),DELHI(I),DELI(I),CIINF(I)
1),EVI(I),LI(I)
  PRINT 170
  170 FORMAT (6X,2HMJ6X,2HAJ16X,2HBJ16X,2HEJ/7)
  DO 180 J=1,JMAX
  180 PRINT 175, MJ(J),AJ(J),BJ(J),EJ(J)
  PRINT 95
  IMAXP1=IMAX+1
  DO 225 I=1,IMAX
  225 PRINT 185, I,(GIL(L,I),L=1,IMAXP1)
  185 FORMAT (4H I=15,23H (GIL(L,I),L=1,IMAX+1)/(3(T/E17.8/7/))

66
190 FORMAT (4H I=1,26H (EPSII(L,I),L=1,IMAX+1)/3(7E18.8/))
195 FORMAT (4H I=15,21H (AIJ(I,J),J=1,JMAX)/5(7E18.8/))
200 FORMAT (4H I=15,23H (ALPI(K,I),K=1,IMAX)/3(7E18.8/))
205 FORMAT (4H I=15,24H (SIGIK(K,I),K=1,IMAX)/3(7E18.8/))
210 FORMAT (4H I=15,23H (AIJ(I,J),J=1,JMAX)/5(7E18.8/))
215 FORMAT (4H I=15,22H (NUIJ(I,J),J=1,JMAX)/5(7E18.8/))
220 FORMAT (4H I=15,23H (NUIJ(I,J),J=1,JMAX)/5(7E18.8/))
225 CONTINUE
230 FORMAT (2X,9HEND INPUT//)
C
C DEFINE SHOCK GEOMETRY
C
C AT EACH X FIND Z S, R S, A CS, COST, SINT AND STORE ON TAPE 10
C
C CALL SHOCKG (DELX, ZTERM, IZTERM)
C
C IZTERM=NUMBER OF DELTA X INCREMENTS AS GENERATED IN SHOCKG
C
IF (NXPST-1.GT.IZTERM) PRINT 235
235 FORMAT (84H NXPST-1. GT. IZTERM, IT MUST BE .LE. FOR PHYSICAL SPACE C
1CALCULATIONS - SEE DO 700 LOOP/) IF (NXPST-1.GT.IZTERM) STOP 301
PRINT 415, IZTERM
IF (IZTERM.GT.50) PRINT 240
FORMAT (1X,50HIZTERM.GT.500 CHANGE DIMENSION OF P.DPDX AND VARI )
IFUZTERM.GT.500) STOP 301
STOP 301
C
C FREESTREAM QUANTITIES
C
SUM=0
DO 245 I=1, IMAX
245 SUM=SUM+C1INF(I)/MUI(I)
MUINF=1./SUM
RHOINF=MUIINF*PINF/(R*TINF)
AINF=SORT(GAMMA*R*TINF/MUIINF)
MINF=VINF/AINF
C
C FOR EACH I, SPECIE
C
EINF=0
DO 275 I=1, IMAX
TEM=EXP(THETAI(I)/TINF)
EVIINF(I)=(R*THETAI(I))/(MUI(I)*(TEM-1.))*FI(I)
C
C FOR EACH L, REACTION LEVEL
C
GSUM=0
GESUM=0
LII=LI(I)
IF (LII.LE.20) GO TO 255
PRINT 250, LII
250 FORMAT (1X,6HLII= I3,2X,28HA LEVEL IN LI ARRAY IS GT 20/2X,43HNEED
1 TO CHANGE DIMENSION OF EPSII AND GIL )
255 CONTINUE
DO 265 L=1, LII
TEM1=EXP(-EPSII(L,I)/TINF)
GSUM=GSUM+GIL(L,I)*TEM1
GESUM=GESUM+EPSII(L,I)*TEM1
IF (LII.LE.20) GO TO 265
PRINT 260, LII, GSUM, GESUM, TEM1, EPSII(L,I), TINF, GIL(L,I)
260 FORMAT (36H I=1, LII, GSUM, GESUM, TEM1, EPSII(L,I), TINF, GIL(L,I)
CONTINUE

EINF = R/MUIM + |EVIINF| + EEIINF + DELHI

IF (IBUG(2).*NE.0) GO TO 275
PRINT 270, IEINF, TEM, THETA(I), TINF, MuI(MUIM) + EEIINF, I, GESUM, GESUM

CONTINUE

PRINT 280, MUINF, RHOINF, AINF, MINF, EIINF, EINF, EEIINF

FORMAT (31H ++ FREESTREAM QUANTITIES ++/8H MUINF=E15.8,10H R
RHOINF=E15.8,8H AINF=E15.8,6H MINF=E15.8,9H EIINF=E15.8,7H E
EINF=E15.8/9H EEIINF=/(8E18.8/)

CONTINUE

PRINT 285, (EIINF(I), I=1,IMAX)

C END FREESTREAM QUANTITIES
C BEGIN QUANTITIES BEHIND SHOCK
C FOR RANGE OF X

PRINT 290

FORMAT (1/33H ++ QUANTITIES BEHIND SHOCK ++/6X,2HTS15X,2HES16X,
12HPS16X,4HRHOS14X,2HUS16X,4HPS1S14X,2HHS)

IF (EOF=10)

IF (NXPST.EQ.0) PRINT 310
IF (NXPST.EQ.0) STOP 2
NXPSTM1=NXPST-1
ITK=0
DO 385 IX=1,IZTERM

C USE RECOUT TO WRITE
C USE RECIN TO READ

CALL RECIN (10),RECIN,X,ZS,RS,RC,COST,SINT)
IF (ENDFILE 10) 295,305

PRINT 300, IE3F

STOP 6
C
C 305 CONTINUE

FORMAT (78H NXPST=2 - SURELY SOME PHYSICAL SPACE VALUES ARE DESIRE
10 -- 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*VINF*SINT
OMEGA=PINF-RHOINF*VINF*2*TEM
DELTA=EINF+PINF/RHOINF+(VINF*2*TEM)/2.
LAMSO=LAMBDA**2
OMEGASO=OMEGA**2
MINF=MINF**2
TEM=TEM-MINF
TG=(TINF*2*GAMMA*TEM-(GAMMA-1.0)*((GAMMA-1.0)*TEM+2.))/<(GAMMA+
1.0)**2*TEM)
IF (IBUG(5).NE.0) GO TO 325
PRINT 320, X,SINT,LAMBDA,OMEGA,DELTA,TEM,TG

FORMAT (39H X, SINT, LAMBDA, OMEGA, DELTA, TEM, TG/7E17.8/)
C C

CONTINUE

DELTTS=10.
APPENDIX A – Continued

E1=0.0001
E2=0.001
MAXI=50
CALL ITR1 (TG,DELTTS,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 I X, I,TEM,EVIS(I)=2I5,2E18.8)
345 SUMG=0.
SUMGE=0.
LII=L1(I)
DO 350 L=1,LII
TEM=EXP(-EPSIIL(L,I)/TS)
SUMG=SUMG+TEM*GIL(L,I)
350 SUMGE=SUMGE+TEM*EPSIIL(L,I)
EEIS=(R/MUI(I))*(SUMGE/SUMG)
EIS=(R*TS/MUI(I))-(FI(I)*R*TS/MUI(I)+1.0*EVIS(I)+EEIS+DELHI(I)

STOP 321

C
C WRITE ON TAPE 11 AT EACH X
CALL RGCOUT (11,1,0,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RGCOUT (11,2,0,EVISd),1=1,IMAX)
C
365 FORMAT (7E18.8)
PRINT 370, IX,(EVIS(I),I=1,IMAX)
370 FORMAT (5H IX=I3,7H EVIS=/4(7E18.3/1/)
375 FORMAT (50H NUMBER OF X-S IN XPS ARRAY,ITK,IS .LT. 3*NXPST/4 - R
1EEXAMINE DELX,NXPST AND XPS ARRAY)
C
380 FORMAT (29H IX,TS,PS,RHOS,US,PSIS,HS,ES/I4,TE18.8)
385 CONTINUE
REWIND 10
END FILE 11
REWIND 11
PRINT 390, ITK,NXPST
390 FORMAT (69H NUMBER OF X-S IN XPS ARRAY,ITK,IS .*LT.* 3*NXPST/4 - R
1EEXAMINE DELX,NXPST AND XPS ARRAY)
C
STOP 301
CONTINUE

69
APPENDIX A – Continued

END COMPUTATION OF QUANTITIES BEHIND SHOCK

CALL FDQDX

FIND PRESSURE, \( P \), AT EACH \( X \) FOR EACH STREAMLINE AND
STORE ON TAPE 9

FIND \( P \) DOT, \( \frac{DP}{DX} \), AT EACH \( X \) FOR EACH STREAMLINE AND
STORE ON TAPE 8

INTEGRATE ALONG EACH STREAMLINE \( \psi \)

\[
\text{VAR}(1) = \text{XVAR}
\]

\[
\text{VAR}(2) = \text{H ENTHALPY}
\]

\[
\text{VAR}(2) \text{ MUST BE } \text{H}, \text{WHICH MAY BE } + \text{ OR } -
\]

\[
\text{CONCENTRATION OF SPECIE}
\]

\[
\text{VAR}(3) = \text{C1(I)}
\]

\[
\text{VAR}(2+\text{IMAX}) = \text{C1(\text{IMAX})}
\]

\[
\text{EQUILIBRIUM VIBRATIONAL ENERGY}
\]

\[
\text{VAR}(2+\text{IMAX+1}) = \text{EV1(1)}
\]

\[
\text{VAR}(2+\text{IMAX+IMAX}) = \text{EV1(\text{IMAX})}
\]

DO 410 \( I = 1, \text{IMAX} \)

TRUNCATE

\[
Y = F1(I) \times (\text{DELI}(I) / \text{THETA}(I) + 1.0)
\]

\[
\text{NI}(I) = \text{AINT}(Y)
\]

IF \((\text{IBUG}(5)) \neq 0) \text{ GO TO 410}

PRINT 405, \( I, Y, \text{NI}(I) \)

405 FORMAT (12H I, Y, NI(I) = I5,2E18.8/)

410 CONTINUE

\[
\text{MU} = 0.
\]

\[
\text{N} = 1 + 2 \times \text{IMAX}
\]

IF \((\text{M} \neq 0)) \text{ N} = \text{N} - \text{IMAX}

PRINT 415, \( \text{IZTERM} \)

415 FORMAT (9H IZTERM=I3, 13)

\[
\text{KSTAG} = 0
\]

\[
\text{ISTAG} = 0
\]

\[
\text{XPST(1)} = \text{DELX}
\]

\[
\text{XPST}(\text{NXPST}) = \text{VAR}(\text{IZTERM}) + 100.0
\]

\[
\text{SUMCl} = 0.
\]

PRINT 95

IZTM1 = IZTERM - 1

LPS1 = 1

IPS1 = 0

BEGIN EACH STREAMLINE COMPUTATION HERE

420 IPSI = IPSI + 1

IF \((\text{IPSI} = \text{EQ} \times \text{IZTERM})) \text{ GO TO 735}

425 CONTINUE

\[
\text{KIPF} = 0
\]

\[
\text{IEOF} = 11
\]

\[
\text{ISTAG = 2 FOR STREAMLINE DELX}
\]

IF \((\text{ISTAG} = \text{EQ} = 1)) \text{ ISTAG} = 2

CALL RECIN (11, 1, IRECIN, IX, TS, ES, PS, RHOS, US, PSIS, MS)

CALL RECIN (11, 2, IRECIN, EISV, 1, IMAX, 1)

IF \((\text{ENDFILE} = 11)) \text{ 430, 440}

430 PRINT 435, \( \text{IEOF}, \text{IPSI} \)

435 FORMAT (5H ENDI4+, 5TH IN MAIN, TRY TO COMPUTE PHYSICAL SPACE VALUES -- IPSI=13/+)

GO TO 735

440 CONTINUE
APPENDIX A – Continued

C
IF ( IPSI.EQ.1) HSTAG=HS
C
CJ=XI
SPEC=Q.0
C EVALUATE DERIVATIVES WHEN SPEC=0.0
II=0
C USE SHOCK VALUES FOR INITIAL COMPUTATION ON EACH STREAMLINE
KEYINF=0
IX=0.
T=TS
IF (I.EQ.0) GO TO 450
DO 445 I=1,IMAX
445 TVI(I)=TINF
DO TO 450
DO 455 I=1,IMAX
455 TVI(I)=TS
460 RHO=RHOS
MU=MUINF
U=US
DO 465 I=1,IMAX
465 MM=2+I
K=IMAX+MM
VAR(MM)=0.
VAR(K)=CIINF(I)
VAR(K)=0.
IF (M.EQ.0) VAR(K)=EVIS(I)
IF (M.EQ.1) VAR(K)=EVIINF(I)
EVH(I)=VAR(K)
CONTINUE
E=ES
H=HS
IF (IPSI.EQ.6.AND.ISTAG.EQ.0) GO TO 635
C
IEOF=9
CALL RECIN (9,IRECIN,X)
CALL RECIN (9,IRECIN,P,IPSI,IZTERM,1)
IF (ENDFILE 9) 430,470
C
470 IEOF=8
CALL RECIN (8,IRECIN,DPDX,IPSI,IZTERM,1)
IF (ENDFILE 8) 430,475
475 IF (IBUG(3).NE.0) GO TO 485
PRINT 480, (VARI(IT),DPDX(IT),P(IT),IT=IPSI,IZTERM)
480 FORMAT (33H (OPOX(IT),P(IT),IT=IPSI,IZTERM) /<6E 17.8 I )
485 CONTINUE
VAR(I)=X
C OMIT PSI=0.0 STREAMLINE FOR NOW — PICK IT UP LATER
IF (X.EQ.0.0) GO TO 490
IG=0
PRINT 725
GO TO 730
C
490 CONTINUE
IF (X.EQ.VARI(IPSI)) GO TO 500
C
PRINT 495, IPSI,X,VARI(IPSI)
495 FORMAT (6H IPSI=14.4H 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 FPDX SUBROUTINE)
STOP 663
C
500 CONTINUE
C
C INITIALIZE
C
STOP 663
C
71
APPENDIX A – Continued

ELB=0
SPEC=0
IF (VAR(I).GT.XPST(I)) LPS1=LPS1+1
LPS2=LPS1
505 CONTINUE

CALL SECOND (CHECKT)

IF (IX.NE.1) GO TO 515
PRINT 510, CHECKT

510 FORMAT (20H ----------- — CHECKT=E15.8 )

515 IF (ICHEK.EQ.1) GO TO 540
IF ((TIMER-CHECKT).GT.30.) GO TO 560
IF (IPS1.GT.5) GO TO 525
PRINT 520

520 FORMAT (IX,/10X,1H$$$$$$$$67H MUST BE ON OR BEYOND PSI=0.;
1 IPS=6, BEFORE PICKUP IS POSSIBLE/10X,10H$$$$$$$/)

525 CONTINUE
KIPF=0
IPF=1

WRITE (13) (XX(I),!=!,8961), (XXX(J),J = 1,28)
WRITE (13) (XXX(J),J = 1,28)

PRINT 530, TIMER, CHECKT

530 FORMAT (30H PICKUP TAPE WRITTEN — TIMER=E15.8,10H CHECKT=E15.8/
1)

ICHEK=1
PRINT 600, IPSI, IX, XVAR, H, MU, PFTL, RHOU, 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,KSTAG

CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
WRITE (13) X,ZS,RS,RC,COST,SINT
CALL RECIN (8,2,IRECIN,DPDX,I,IZTERM,1)
WRITE (13) (DPDX(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,1,IZTERM,1)
WRITE (13) X
WRITE (13) (P(J),J=1,IZTERM)

545 CONTINUE
DO 550 I=1,KSTAG

CALL RECIN (12,1,IRECIN,IPSIRHOURT,VAR(I),PSIS)
WRITE (13) IPSIRHOURT,VAR(I),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 ---/)

72
APPENDIX A - Continued

560 CONTINUE
   IX=IX+1
C
C    CALL CALINTH (VAR,DER,ELE1,ELE2,CJ,SPEC,N,CUVAR,ELB,CIMAX,NERR,PHM
1AX)
C
IF (NERR.EQ.0) GO TO 575
IF (NERR.EQ.1) PRINT 565, CJ,N
565 FORMAT (16H BAD INPUT,CJ,N=E17.8,15)
IF (NERR.EQ.2) PRINT 570, ELE1,ELE2
570 FORMAT (IX=21H EXAMINE ELE1 AND ELE2/1G(7E17.8/))
IF (NERR.EQ.1.OR.NERR.EQ.2) STOP 665
KIPF=KIPF+1
IF (KIPF.NE.IPF) GO TO 625
KIPF=0
C
575 CONTINUE
IF (IX.EQ.1) GO T0 580
IF (IPS1.LE.6.AND.IX.EQ.6) GO TO 530
IF (VAR(l).GE.VARKIZTERM) ) GO TO 580
IF (IPS1.LT.6.AND.VAR(l).GE.DELX) GO TO 580
KIPF=KIPF+1
IF (KIPF.NE.IPF) GO TO 625
KIPF=0
C
580 CONTINUE
IMAXP2=IMAX+2
SUMCI=0.
DO 590 ISUM=3,IMAXP2
   IF (VAR(ISUM).LT.0.) NEG=-1
   IF (VAR(ISUM).LT.0.) PRINT 535
   585 FORMAT (/5X.21H NEGATIVE CI=0/)
   SUMCI=SUMCI+VAR(ISUM)
   DO 595 ICM=1,IMAX
      C
C      PRINT ANSWERS
C
      CMUCM) = VARUCM+2)*MU/MUKICM)
      PRINT 600, IPSI,IX,XVAR,H,MU,PFTL,RHC,U,T,E,SPEC,SUMCI
      600 FORMAT (2XI 2.15.8X,2HX=015.8,7X,2HH=D15.8,7X,3HMU=E15.8,7X,2HP=E15
0.8,7X,2HRO=E15.8,7X,2HE=E15.8,5X,3HC1 =2E15.8,1X,8HSUM(CI)=E15.8)
      PRINT 605, (VAR(I),I=3,IMAXP2)
      605 FORMAT (10X.9H CI( 11)=E15.8,9H CI( 21)=E15.8,9H CI( 31)=E15.8,9H
1 CI( 41)=E15.8,9H CI( 51)=E15.8/10X,9H CI( 61)=E15.8,9H CI( 71)=E15.
2,9H CI( 81)=E15.8,9H CI( 91)=E15.8,9H CI(101)=E15.8/10X,9H CI(11
31)=E15.8,9H CI(12)=E15.8,9H CI(13)=E15.8,9H CI(14)=E15.8,9H CI(15
1)=E15.8/10X,9H CI(16)=E15.8,9H CI(17)=E15.8,9H CI(18)=E15.8,
3 CI(19)=E15.8/10X,9H CI(20)=E15.8/10X,9H CI(21)=E15.8,9H CI(22)=
500.9H CI(23)=E15.8,9H CI(24)=E15.8,9H CI(25)=E15.8
1 PNT 610, (CM(I),I=1,IMAX)
1 CM( 41)=E15.8,9H CM( 51)=E15.8/10X,9H CM( 61)=E15.8,9H CM( 71)=E15.
2,9H CM( 81)=E15.8,9H CM( 91)=E15.8,9H CM(101)=E15.8/10X,9H CM(11
31)=E15.8,9H CM(12)=E15.8,9H CM(13)=E15.8,9H CM(14)=E15.8,9H CM(15
1)=E15.8/10X,9H CM(16)=E15.8,9H CM(17)=E15.8,9H CM(18)=E15.8,
3 CM(19)=E15.8/10X,9H CM(20)=E15.8/10X,9H CM(21)=E15.8,9H CM(22)=
500.9H CM(23)=E15.8,9H CM(24)=E15.8,9H CM(25)=E15.8
1 IMAXL=2+IMAX+1
IMAXP3=2+IMAX+1
1 PNT 615, (VAR(I),I=IMAXP3,IMAXL)
      615 FORMAT (10X,9H EVI( 1)=E15.8,9H EVI( 2)=E15.8,9H EVI( 3)=E15.8,9H
2 ,9H EVI( 8)=E15.8,9H EVI( 9)=E15.8,9H EVI(10)=E15.8/10X,9H EVI(1
31)=E15.8,9H EVI(12)=E15.8,9H EVI(13)=E15.8,9H EVI(14)=E15.8,9H EVI
4(15)=E15.8/10X,9H EVI(16)=E15.8,9H EVI(17)=E15.8,9H EVI(18)=E15.8,
APPENDIX A – Continued

59H EVI(19) = D15.8, 9H EVI (20) = D15.8, 9H EVI (21) = D15.8, 9H EVI (22) =
6015.8, 9H EVI (23) = D15.8, 9H EVI (24) = D15.8, 9H EVI (25) = D15.8

PRINT 620
620 FORMAT (/)
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
WHEN IPSI = 6, DELX AND STAGNATION STREAMLINES WILL BE COMPUTED
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. 0 OR ISTAG .EQ. 2) GO TO 690
C
ISTAG = 0 UNTIL AFTER EXTRAPOLATION FOR PSI = 0. STREAMLINE
C
ISTAG = 1 FOR PSI = 0.0 STREAMLINE
C
ISTAG = 2 FOR DELX STREAMLINE AND THEREAFTER
C
635 CONTINUE
IG = IG + 1
IGC = 0
IGE = IMAX + 2
PSIG (IG) = PSI S
DO 640 IG1 = 3, IMAX + 2
IGC = IGC + 1
CIG (IGC, IG) = VAR (IG1)
IGE = IGE + 1
EG (IGE, 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 330
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)
645 EIT (IG1) = EIG (IG2, IG1)
CALL FTLUP (PSI, CI (IG2), MG, IG, PSIG, CIT)
IF (CIT (IG2) .LT. 0.0) CIT (IG2) = 0.00000001
CALL FTLUP (PSI, EVI (IG2), MG, IG, PSIG, EIT)
I3 = IMAX + 1
EG (I3, IG) = EVI (IG2), PSIG
646 FORMAT (215/7E17.8)
650 VAR (2*IMAX + I2) = EVI (IG2)
DO 655 IG1 = 1, 6
CALL RECIN (10.1, IRECIN, X, ZS, RS, RC, COST, SINT)
655 CONTINUE
C
INITIALIZE FOR PSI = 0. STREAMLINE
C
CJ = XI
SPEC = 0.0

74
APPENDIX A – Continued

II=0
KEYINT=0
IX=0
SUM=0
DO 660 1=1,IMAX
SUM=SUM+CH(I)/MUH(I)
IF (EVI(I).EQ.0.) TVI(I)=0.
IF (EVI(I).EQ.0.) GO TO 660
XL=(DGENK(I)*R*THETAI(I))/(MUH(I)*EVI(I))+1.0
ALN=ALOG(XL)
TVI(I)=THETAI(I)/ALN
660 CONTINUE
PRINT 661,(EVI(I),TVI(I),I=1,IMAX)
661 FORMAT(5X,D17.8,E17.8)
C
U=SORT(2.0*(HSTAG-H))
C
VAR(1)=OELX
C COMPUTE P AND DPCX AT IPSI=6
PRINT 665
665 FORMAT (24H PSI=0.000 STREAMLINE—>
PS(6)=PS+US/(RC*RS)*(-PSIS)
RHO(6)/H-E
DO 670 I=7,IZTERM
CALL RECIN (11,1,RECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,RECIN,EVIS,1,IMAX,1)
CALL RECIN (10,1,RECIN,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 OPDX(n = OIF<LG,MG,NPG,VARI(6),P(6))
DO 680 I=1,5
CALL RECIN (11,1,RECIN,IX,TS,ES,PS,RHOS,US,PSIS,HS)
CALL RECIN (11,2,RECIN,EVIS,1,IMAX,1)
680 CONTINUE
ISTAG=1
PSIS=0.
CALL SECOND (CHECKT)
PRINT 685, CHECKT
685 FORMAT (1<>H CHECKT=E15.8,6H /)
PRINT 686,(EVI(I),I=1,IMAX)
686 FORMAT(7D17.8)
GO TO 500
C
690 CONTINUE
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)
RHOURT=1./RHO*U
IF (IBUG(13).NE.0) GO TO 700
PRINT 695, IPSI,RHOURT
695 FORMAT (7H IPSI=I3,9H RHOURT=E15.8)
700 CONTINUE
CALL RECOUT (12,1,0,IPS1,RHOURT,VAR(1),PSIS)
GO TO 715
705 YPSIS=PREPSIS+XPST(LPS2)-PREX)*((PSIS-PREPSIS)/(VAR(1)-PREX))
RHOURT=PRERU+(XPST(LPS2)-PREX)*((RHO*U-PRERU)/(VAR(1)-PREX))
RHOURT=1./RHOURT

75
CALL RECOUT (12,1,0,IPSI,RHOURT,XPST(LPS2),YPIS)
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=214,33H X,XPST,PREPSIS,PSIS,PRERU,PREX=/01
17.8,3E17.8)
715 CONTINUE
LPS2=LPS2+1
KSTAG=KSTAG+1
720 CONTINUE
PRES=VAR(1)
PRERU=RHO*U
PREPSIS=PSIS
IF (VARI .LT. VARI (IZTERM) ) GO TO 505
C FINID 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 635, CHECKT
REWIND 8
REWIND 9
REWIND 10
REWIND 11
PRINT 740, KSTAG
740 FORMAT (137H BEGIN PHYSICAL SPACE CALCULATIONS AT,I5.10H 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)
755 FORMAT (18H LPS,X,XPST(LPS) I5,2E30.15/)
760 CONTINUE
IF (ABS(X-XPST(LPS))*GT.1.E-8) GO TO 745
IF (IBUG(13) .NE. 0) GO TO 765
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.E-8) GO TO 780
IK=IK+1
IF (IK .GE. 200) PRINT 770, IK
770 FORMAT (1X,50H IK .GE. 200, CHANGE DIMENSION OF RUT AND PSISTG, IK=,I13)
    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
C
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
   CONTINUE
C TRUNCATE
   L=INT(XDEL)!
C REMAINDERING
   M=MOD(L,2)
   IF (M.NE.O) 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)
   LM=L-1
   IF (IBUG(13).NE.O) GO TO 795
   PRINT 790, L,SMALL,XDEL,DPSIS,RB
  790 FORMAT (25H L,M,SMALL,XDEL,DPSIS,RB/2I5,*E17.8)
   CONTINUE
   DO 800 I=2,L,2
   PSII=PSII+DPSIS
   CALL FTLUP (PSI I,RUT,1,IK,PSISTG,RUT)
   IF (I.EQ.L) RB=RB+4.*RUT
   IF (I.EQ.L) GO TO 800
   PSII=PSII+DPSIS
   CALL FTLUP (PSI I,RUT,1,IK,PSISTG,RUT)
   RB=RB+4.*RUT+2.*RUT
  800 CONTINUE
C
   RB=RB*DPSIS/3.
   IF (IBUG(13).NE.O) GO TO 810
   PRINT 805, RB,RS,COST,RB,SINT
  805 FORMAT (21H RB,RS,COST,RB,SINT=5E17.8)
   CONTINUE
   ARR=SORT(RS**2-2.*COST*RB)
   YI=(RS-ARR)/COST
   ZE=ZS+YI*SINT
   PRINT 815, X,ARR,YI,ZE,PSISTG(IK)
  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
C
   IF (IBUG(13).NE.O) GO TO 825
   PRINT 820, TR,RB
  820 FORMAT (5HTR,RB,2E17.8)
   CONTINUE
   ARR=SORT(RS**2-2.*COST*RB)
   YI=(RS-ARR)/COST
   ZE=ZS+YI*SINT
   PRINT 815, X,ARR,YI,ZE,PSISTG(IK)
  830 CONTINUE
   PRINT 835
  835 FORMAT (7/)
C
   CONTINUE
   CONTINUE
   PRINT 850
  850 FORMAT (29H END THIS CASE, HALLELUJAH)
SUBROUTINE BASIC

BASIC CALLED BY CALINTH TO EVALUATE DERIVATIVES H DOT, C SUB I DOT AND EV SUB I DOT

DERIVATIVES START IN DER(I)

COMMON M,IX,IMAX,IPS1,IBUG(15)
COMMON P(500),DPDX(500),VARI(500)
COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIIINF(25), 1 LI(25)
COMMON R,MUIINF,DELTA,LAMSQ,OMEGSQ,OMEGA,MU,T,U
COMMON EPSII(20,25),GII(20,25)
COMMON VAR(52),CUVAR(52),DER(51)

COMMON IS,RS,C,SINT,COST,PS,US,PSIS
COMMON MJ(50),EI(50),AJ(50),BI(50)
COMMON TVI(25),NI(25),OGENI(25)
COMMON NUIJ(26,50),AIJ(25,50),NUPIJ(25,50)
COMMON SIGI(25,25),ALPI(25,25)

COMMON /LAB2/ DELX,ZISTERM,IRESULT
COMMON /LAB3/ EINF,PINF,RHOINF,VINF,E,JMAX,KEYINT,RHO,HSTAG
COMMON /LAB4/ PFTL,KI,KM,EITR1
COMMON /LAB5/ IUNEG
COMMON /LAB7/ ITNEG,IEXP

DOUBLE PRECISION VAR
DIMENSION PHI(50),KJ(50),SJ(50)
DIMENSION CI(25),EVI(25),DCIDX(25),DEVIDX(25),EVI BAR(25)

EQUIVALENCE (CUVAR(2),H),(CUVAR(3),EI(1))
EQUIVALENCE (DER(1),DHDX),(DER(2),DCIDX(1))

REAL KJ,LAMSQ,MU,MUI,NI,NIJ,NUPIJ

DER(1)=DHDX MUST BE DHDX AS H MAY BE + OR -
DER(2)=DCIDX(1)

DER(1+IMAX)=DCIDX(IMAX)
DER(1+IMAX+1)=DEVIDX(1)
DER(1+IMAX+IMAX)=DEVIDX(IMAX)

CUVAR(1)=X
CUVAR(2)=H*ENTHALPY - IT MUST BE H WHICH MAY BE + OR -
CUVAR(3)=CI(1)

CUVAR(2+IMAX)=CI(IMAX)
CUVAR(2+IMAX+1)=EVI(1)
CUVAR(2+IMAX+IMAX)=EVI(IMAX)

EXTERNAL FOFE
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 CONTINUE
INTERPOLATE FOR P ACROSS INTEGRATION INTERVAL
DO 15 I=1,IMAX
EVI(1)=CUVAR(2+IMAX+1)
MFTL=1
NFTL=IRESULT-IPS1+1
CALL FTLUP (CUVAR(1),PFTL,MFTL,NFTL,VARI(IPS1),P(IPS1))
APPENDIX A — Continued

C INTERPOLATE FOR DPOX
CALL FTLP (CUXAR(1),OPXFL,FTFL,NFTL,VARI(IPS1),DPOX(IPS1))
IF (IBUGU(O).NE.0) GO TO 30
PRINT 20, E,FTFL,P(IPS1),P(IPS1+1),CUXAR(1),DPOX(IPS1)
20 FORMAT (25H E,FTFL,P(IPS1),P(IPS1+1),CUXAR(1))
PRINT 25, (CH 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)/MVH(I)
IF (EVI(I).EQ.0.) TVI(I)=0.
IF (EVI(I).EQ.0.) GO TO 35
XL=(DGENI(I)*R*THETAI(I))/(MVH(I)*EVI(I))+1.0
ALN=ALOG(XL)
TVI(I)=THETAI(I)/ALN
35 CONTINUE
IF (IBUG(10).GT.0) GO TO 45
PRINT 40, I,DGENI(I),R,THETAI(I),MVH(I),EVI(I),XL,ALN,TVI(I)
40 FORMAT (26H I,DGENI, R, THETA I, MV H, EV I, 15.8, / 11H XL, ALN, TV I / 18.8, /)
45 CONTINUE
MU=1.0/0
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, I.CODE= 12 »
IF (ICODE.NE.1) STOP 66
C WHEN ICODE=1, TRY A NEW STARTING E, DO THIS 2 TIMES
IF (ICODE.EQ.3) STOP 66
E=EITR1
KCODE=KCODE+1
GO TO 55
75 CONTINUE
IF (ICODE.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
RH0=PFTL/(1-H)
T=(PFTL*MU)/(RH0*R)
IF (T.GT.0.0) GO TO 95
PRINT 90, T,RH0,PFTL,H,E,MU
90 FORMAT (14H T NEGATIVE =E15.8,2X,4HRHO=E15.8,2X,3HPFTL=E15.8,2X,2
1HE=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,RH0,T,MU,U,H
100 FORMAT (16H I X,IPSI,RHO,T=214,4E17.8,E17.3/)
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 (FJ(IJ).NE.0.0) GO TO 120
115 PHI(J)=1.0
GO TO 125
120 CONTINUE
TEM=EXP(THETAI(I)/TVI(I))
TEM1=EXP(THETAI(I)/T)
TEM2=EXP(-NI(I)*THETAI(I)/TVI(I)-THETAI(I)/T))
TEM3=EXP(THETAI(I)/TVI(I)-THETAI(I)/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)/NII(I)
125 TEM4=EXP(-EJ(J)/T)
C KJ = RATF CONSTANT
KJ(J)=AJ(J)*T**8.8*J(J)*TEM4
IF (MUJ(J)*IMAX+1.EQ.0.) SJ(J)=1.0
IF (MUJ(J)*IMAX+1.EQ.0.) GO TO 140
SUM=0.
DO 135 ISUM=1,IMAX
C
SUM=SUM+AJ(J)*ISUM+MUI(I)*SUM+AJ(I)*ISUM
IF (IBUG(7).NE.0) GO TO 135
PRINT 130, 1,J,ISUM,SUM,AJ(J)*ISUM+MUI(I)
130 FORMAT (25H I,J,ISUM,SUM,AJ(J),CI+MUI/I315,5E17.8/
C
135 CONTINUE
SJ(J)=RH0*SUM
140 CONTINUE
IF (IBUG(7).NE.0) GO TO 150
C
80
```
APPENDIX A – Continued

PRINT 145, I, J, FI(IJ), 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, TEM2/215, 5E18.8/22H TEM3, TEM4, AJ
1, BJ(J), 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/MUH(IPROD)
IF (TEM.GE.D) GO TO 165
C LET PROBLEM COMPUTE THRU DERSUB WHEN CI NEG.
C MAKE DECISION IN MAIN ABOUT ACCEPTING NEG CI
ABW=AMOD NUJ(IPROD, J, 2.0)
IF (ABW.EQ.0.0) GO TO 170
IF (TEM.LT.0.0) PRINT 155, I, J, IX, PROD, TEM, RHO, MUJ(IPROD), NUIJ(IPROD)
100, J, CI(IPROD), PROD, ABW
155 FORMAT (2X, 32H I, J, IX, IPROD, TEM, RHO, MUJ, 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, 6E117.8)
180 CONTINUE
DCIJDX=PHI(J)*KJ(J)*SJ(J)/(MUI(I)/(RHO)*U*WUJ(I, J), NUIJ(I, J), PROD, DCIDX(I)
185 FORMAT (25H I, J, DCIJDX, PHI(J, KJ(J, SJ(J, MUI(I), RHO, U, NUIJ(I, J), N
1UJ(I, J), PROD, DCIDX(I)
190 CONTINUE
TEM=EXP(THETA(I)/T)
TEM1=(FI(I)*OGEN(I)*R*THETA(I))/MUI(I)
EVBAR(I)=TEM1/(TEM-1.0)
IF (M.NE.0) GO TO 195
VAR(I+IMAX+2)=EVBAR(I)
DEVIDX(I)=0.
GO TO 210
195 CONTINUE
TAUSUM=0.
IF (FI(I).EQ.0.0) GO TO 210
DO 205 K=1, IMAX
TEM3=EXP(-THETA(I)/T)
TEM4=EXP(SIGIK(K, I)*T**(1.0/3.0))
TEM5=FI(I)*ALPIK(K, I)/PFTL
TAUIK=TEM5*(T**BETA(IK(K, I)*TEM4/1.0-TEM3)
TEM6=CI(K)*EVBAR(I)-EVWI(I)
TAUSUM=TAUSUM+TEM6/TAUIK(K)
C
81
APPENDIX A – Continued

IF (IBUG(9) .NE. 0) GO TO 205
PRINT 200, I, K, TEM3, TEM4, TEM5, TAU1K, TAU5UM, SIGIK(K, I), ALPIK(K, I),
1 ETAIK(K, I), U, EV1, EV2BAR, TEM1, TEM2, TEM6, TEM6
200 FORMAT (33H, I, K, TEM3, TEM4, TEM5, TAU1K, TAU5UM/215, 5E18.8/33H, SIGIK
1, ALPIK, ETAIK, U, EV1, EV2BAR/6E17.8/22H, TEM1, TEM2, TEM6/4E18.8
2.022/1)
205 CONTINUE
C
C DEVIDX = EQUILIBRIUM VIBRATIONAL ENERGY
DEVIDX(I) = TAU5UM
DER(I+IMAX+1) = DEVIDX(I)
210 CONTINUE
C
C COMPUTE OHDX
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, OPOX, OHOX=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 PI(500), DPDIK(500), VARI(500)
COMMON EV1INF(25), THETAI(25), MUI(25), FI(25), DELHI(25), CIINF(25),
1 LI(25)
COMMON R, MUI, DELTA, LAMSAQ, OMESQ, OMEGA, MU, T, U
COMMON EPSIIL(20, 20), GIL(20, 20)
COMMON VAR(52), CVAR(52), DER(51)
COMMON /LAB*/ PFTL, KITR1, EITR1
COMMON /LAB7/ ITNEG, IEXP
C
C DOUBLE PRECISION VAR
C
C DIMENSION CI(25)
C
C EQUIVALENCE (CUVAR(3), CI(1)), (CUVAR(2), H)
C
C REAL MUI, LAMSAQ, 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, PHO, PFTL, H
5 FORMAT(1X, 5HEOUM=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
35 CONTINUE

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APPENDIX A — Continued

```
TEM = EXP(THETA(I)/TVI(I))
TEM1 = (1.5*R*T)/MUI(I) + (FI(I)*R*T)/MUI(I) + (FI(I)*R*THETA(I))/(MUI(I)*TEM-1.0))
15 CONTINUE
SUMG = 0.
SUMGE = 0.
C
LIIL = LI(I)
DO 25 L = 1, LIIL
TEM3 = EPSIIIL(L, I)/T
IF (TEM3.LT.741.67) GO TO 42
PRINT 41, TEM3, EPSIIIL(L, I), T, EDUM(L, I), H, MU, KITR1
41 FORMAT (56H EXPCTEM), TEM3 .GT .741.67, TEM3.EPSIIIL (L, I), T, EDUM, L, I =
1 /6E17.8, 215, 13H, H, 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)*EPSIIIL(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, EPSIIIL(L, I), T, SUMG, GIL(L, I), SUMGE
20 FORMAT (34H I ,L , 1 EP2 ,EPSI I L, T,SUMG.GI L,SUMGE/2I5,6E18.8/)
25 CONTINUE
IF (SUMGE.LT.10.E3GC) GO TO 26
PRINT 27
C
27 FORMAT (56H IN FCFE, SUMGE.GT. 10. E300, SET IEXP=1 TO REDUCE INTERVAL)
C
IBUG(11) = 1
IEXP = 1
RETURN

26 CONTINUE
EI = TEM1 + R/MUI(I)*(SUMG/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, RHQ, T, TEM, TEM1, SUMG, SUMGE, EI,
1E
30 FORMAT (32H I ,L , IX, IPSI, PORHO, E, EDUM, H, RHQ/4I4, 6E18.8/23H T,TEM,
1TEM1, SUMG, SUMGE/7E18.8//)
35 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(CU)
C CALLED BY ITR1 IN MA IN PROGRAM TO EVALUATE TS
C
COMMON M, IX, IMAX, IPSI, IBUG(15)
COMMON PHI(500), DPDX( 500), VARI( 500)
COMMON EVIINF(25), T*ETA(I)(25), MUI(25), FI(25), DELHI(25), CIINF(25),
1 L(25)
COMMON R, MUIINF, DELTA, LAMSQ, OMEGASQ, OMEGA, MU, T, U
COMMON EPSIIIL(20, 2C), GIL(20, 20)
COMMON VAR(52), CUVAR(52), DER(51)
```
APPENDIX A – Continued

DOUBLE PRECISION VAP
C
DIMENSION CI(25)
C
EQUIVALENCE (CUVAR(3),CI(1))
C
REAL MUI,LAMSQ,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))/CUM
  EVIS=(R*THETA(I))/ (MUI(I) )*( TEM-1.0 )*FI(I)
  SUMG=0
  SUMGE=0
C
  LII=LII(I)
  DO 10 L=1,LII
    TEM1=EXP(-EPSIIL(L,I)/DUM)
    SUMG=SUMG*TEM1*GIL(L,I)
  SUMGE=SUMGE*TEM1*GIL(L,I)*EPSIIL(L,I)
  EEIS=(R/MUI(I))*(SUMG/SUMGE)
  EVIS=(R/MUI(I))*(SUMG/SUMGE)
  ES=ES*EIS*CIINF(I)
  IF (IBUG(4).NE.0) GO TO 20
C
  T=DUM
  PRINT 15, IX,I,M,EVIS,TEM,T,SUMG,SUMGE,TEM1,EEIS,EIS,ES,CIINF(I)
  FORMAT (32H, IX,I,M,EVIS,TEM,T,SUMG,SUMGE,TEM1,EEIS,EIS,ES,CIINF(I)
  1)
C
  20 CONTINUE
  25 CONTINUE
C
  FAC=SQRT(OMEGS*2*LAMSQ*(DELTA-ES))
  FIN=(2.*MUINF*(DELTA-ES)*FAC)/(R*(OMEGA*FAO)
  FOFTS=FIN
  IF (IBUG(4).NE.0) RETURN
  PRINT 30, OMEGS,LAMSQ,DELTA,ES,MUINF,FAC,R,OMEGA,FIN
  FORMAT (44H, OMEGS,LAMSQ,DELTA,ES,MUINF,FAC,R,OMEGA,FIN/215E18.8/)
  1)
  RETURN
END
SUBROUTINE FDPCX
C
TO COMPUTE P AND CFCX
AND SAVE ON TAPES 9 AND 8
C
COMMON M,IX,IMAX,IPS,IBUG(15)
COMMON P( 500),DPCX( 500),VAR( 500)
COMMON EVIINF(25),THETAI(25),MUI(25),FI(25),DELHI(25),CIINF(25),
  1
LII(25)
COMMON R,MUIN,DELTA,LAMSQ,OMEGS,CMEGS,CMEG,CMEG,MT,CMOMEN
COMMON EPSIIL(25,2C),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 T(25),HI(25),DENH(25)
COMMON MUIJ(21,20),AIIJ20,30,NUPI2(20,33)
COMMON SIGIK(20,20),ALPIK(20,20),BIETAIK(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)

COMMON /LAB2/ CELX, ZSTERM, IZTERM

DOUBLE PRECISION

C
C BEGIN PRESSURE DISTRIBUTION
C FOR EACH PSI FIND RANGE OF X

DO 20 IPSI=1,IZTERM
DO 15 IX=1,IZTERM
IEOF=10
CALL RECIN (10,1,IRECIN,X,ZS,RS,RC,COST,SINT)
IF (IEOF,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 (IEOF,11) 75,10
10 CONTINUE
IF (IXT.LT.IPSI) GC TO 15
IF (IXT.EQ.IPSI) PSISHK=PSIS
IF (IPSI.EQ.IX) P(I)=PS
IF (IPSI.EQ.IX) GC TO 15
P(I)=PS+US/(RC*RS)*(PSISHK-PSIS)
15 CONTINUE
REWIND 10
REWIND 11

CALL RECOUT (9,1,0,XX)
CALL RECOUT (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 (IEOF,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(I+2)=0.0
ITHIS=ITHIS+1
VARI(ITHIS)=XT
40 CONTINUE
WHERE=0
C
DO 60 IX=IPSI,IZTERM
IF (IX.EQ.IZTERM) P(I+1)=0.
IF (IX.EQ.IZTERM) P(I+2)=0.0
WHERE=WHERE+1
C DIFFERENTIATE
IF (IX.NE.IPSI) GC 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) GC TO 50

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APPENDIX A – Continued

\texttt{DPDX(IX) = (P(IX-2) - 4 \cdot P(IX-1) + 3 \cdot P(IX)) / (2 \cdot CELX)}

\texttt{CONTINUE}
\texttt{IF (IBUG(1).NE.0) GC TO 60}
\texttt{PRINT 55, IPSI, IX, A, DPDX(IX), P(IX)}
\texttt{CONTINUE}
\texttt{C}
\texttt{CALL RECOUT (8,2,0,DPDX,IPSI,IZTERM,1)}
\texttt{CONTINUE}
\texttt{DO 70 IX = 1, IZTERM}
\texttt{IF (IX.EQ.1) VARI(1) = 0.}
\texttt{IF (IX.EQ.1) GO TO 7C}
\texttt{IF (IX.LT.7) VARI(IX) = VARI(IX-1)+DELX/5.}
\texttt{IF (IX.GT.6) VARI(IX) = VARI(IX-1)+DELX}
\texttt{CONTINUE}
\texttt{REWIN 9}
\texttt{REWIN 10}
\texttt{REWIN 11}
\texttt{STOP}
\texttt{FORMAT(7H EOF 15, 13H IN FDPDX)}
\texttt{STOP 50}
\texttt{END}

SUBROUTINE CHECK

CHECK CALLED BY CALINTH TO MAKE DECISION TO ACCEPT ANSWERS

\texttt{IF ACCEPTABLE, SET ELB=0 AND RETURN}

\texttt{IF NOT ACCEPTABLE MODIFY SPEC AND CI. SET ELB=1.0 AND RETURN}

\texttt{COMMON M, IX, IMAX, IPSI, IBUG(15)}
\texttt{COMMON P(500), DPDX(500), VARI(500)}
\texttt{COMMON EVINI(25), THETAI(25), MUI(25), FI(25), DELHI(25), CIAINF(25),}
\texttt{LI(25):}
\texttt{COMMON R, MUIINF, DELTA, LAMSQ, CMEGSQ, OMEGA, MU, T, U}
\texttt{COMMON EPSIIH20.2C), GIL(20,20)}
\texttt{COMMON VAR(52), CUVAR(52), DER(51)}
\texttt{COMMON /LAB6/ ELB, SPEC, CJ, TPREV, HPREV, HCHECK, TCHECK}
\texttt{COMMON /LAB7/ ITNEG, IEXP}
\texttt{EQUIVALENCE (CUVAR(2), H)}
\texttt{DOUBLE PRECISION VAR}
\texttt{IF (IEXP.NE.1) GO TO 1}
\texttt{GO TO 15}
\texttt{REDUCE COMPUTING INTERVAL TO TRY TO AVOID EXP ERROR STOP}
\texttt{CONTINUE}
\texttt{IF (ITNEG.EQ.0) GC TO 4}
\texttt{E.GT.H LEADS TC NEG T SOMETIMES---LETS REDUCE INTERVAL TO TRY}
\texttt{TO AVOID INSTABILITY}
\texttt{GO TO 15}
\texttt{CONTINUE}
\texttt{IMAXP1 = IMAX+1}
\texttt{DO 10 I = 3, IMAXP1}
\texttt{CLVAR(2) = H MAY BE NEG}
\texttt{IF (CUVAR(1).LT.0.) PRINT 9, 1, IX, CUVAR(1)}
\texttt{CONTINUE}
\texttt{IF (IX.LT.2) GC TO 30}
\texttt{IF (IPSI.EQ.6.AND.IX.LT.8) GC TO 30}
\texttt{IF (ABS(TPREV-T)/T.LT.TCHECK) GC TO 25
APPENDIX A – Continued

CONTINUE
    IF(SPEC.LT.1.0E-15) STOP 30
C REDUCE INTERVAL
    SPEC=SPEC/4.
    CJ=SPEC
    ELB=1.0
    PRINT 44,SPEC,IPSIX,T,TPREV,H,HPREV,IEXP,ITNEG
44 FORMAT(35H REDUCED SPEC=E15.8,10H IPSI , IX=2I5, 18H T , TPREV H, HPRE
    IV=4E16.7/12H IEXP,ITNEG=2I3)
    ITNEG=0
    IEXP=0
    RETURN
25 CONTINUE
    IF(ABS((HPREV-H)/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)
C SUBROUTINE SHOCKG CALLED BY MAIN
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 USER MUST STORE THE NUMBER OF X VALUES IN IZTERM
C USE STOP 13 FOR ERROR STOPS IN SHOCKG
C
DIMENSION 2DUM(1000),RSDUM(1000),RCDUM(1000),SIDUM(1000),
1 CODUM(1000),XC(1000)
C
C NEQ A 12-16-66
C Z/L=COS(R/L)-1.0
C L=2.109211 CM
C NEQZ INPUT
C
E L=2.109216
X=0.
DRS=.0078125
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(RCDUM(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(CRS)**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)
ZDUM(NRS) = EL*ZDUM(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 LE 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, SIDUM)
PRINT 35, X, ZS, RS, RC, COST, SINT, NOX
35 FORMAT (6E17.8, I5)
CALL RECON (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
STOP 13
STOP 13
C

SUBROUTINE CALINTH(VAR, DER, ELE1, ELE2, CI, SPEC, N, CUVAR, ELT,
ICIMAX, NERR, PHMAX)
C
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(51), DER(51), ELE1(51), ELE2(51), CUVAR(52), ELT,
ICIMAX, NERR, PHMAX)
C
C NERR=1 CI OR N IS EQUAL TO ZERO
C NERR=2 ELE1 LESS THAN OR EQUAL TO ELE2
C
C TEST INPUT
C
FN = N
TEST = CI*FN
997 NERR = 1
RETURN
998 IF (ELE1-ELE2)999, 998, 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 = N1 + 1
DO 3 I = 1, N1
3
APPENDIX A – Continued

3 CUVAR(I) = VAR(I)
   CALL BASIC
   RETURN WITH DERIVATIVES IN DER

   DO 4 I = 1, N
     4 F1(I) = DER(I)
   DO 7  I = 1, N
     Y2(I) = VAR(I) + CI/2. * F1(I)
     IF(I .EQ. 1) GO TO 6
     IF(Y2(I)) .LT. 6.6, 6.6
       CUVAR(I) = Y2(I)
       GO TO 66
   65 SPEC = CI
     CI = CI/2.
     GO TO 5

66 CALL BASIC TO EVALUATE F2
   CALL BASIC
   RETURN

   DO 7 I = 1, N
     F2(I) = DER(I)
   DO 9 I = 1, N
     Y3(I) = VAR(I) + CI/2. * F2(I)
     IF(I .EQ. 1) GO TO 7
     IF(Y3(I)) .LT. 7, 7
       CUVAR(I) = Y3(I)
   CALL BASIC TO EVALUATE F3
   CALL BASIC
   RETURN

   DO 10 I = 1, N
     F3(I) = DER(I)
   COMPUTE P, PH AND CAP F TERMS

      IF(Y3(I)) .LT. Y2(I)) 5, 8, 9
      P(I) = 0.
      GO TO 91
     9 P(I) = -((F3(I) - F2(I)))/(Y3(I) - Y2(I))
     PH(I) = P(I) * CI
     IF(PH(I)) .LT. 83, 83, 103
      PH(I) = 0.
      P(I) = 0.
      GO TO 84
   83 PH(I) = 0.
   91 GO TO 84
   103 IF(ABS(Y3(I) - Y2(I))/((ABS(Y3(I)) + ABS(Y2(I))))/2.) .LT. 5E-4) 83, 83, 84
   84 IF(PH(I)) .LT. 85, 85, 85
   85 CAPF1(I) = 1. - PH(I)/2. + (PH(I)**2)/6. - (PH(I)**3)/24.

89
APPENDIX A - Continued

\[
\text{CAPF2}(I) = \frac{5}{6} \text{PH}(I) + \frac{(\text{PH}(I)^2)}{24} - \frac{(\text{PH}(I)^3)}{120}.
\]

\[
\text{CAPF3}(I) = \frac{1}{6} \text{PH}(I) - \frac{(\text{PH}(I)^2)}{24} + \frac{(\text{PH}(I)^3)}{120} - \frac{(\text{PH}(I)^4)}{720}.
\]

\[
= \frac{1}{6} - \frac{\text{PH}(I)}{24} + \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF3}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF1}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF2}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF3}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CONTINUE}
\]

\[
\text{GO TO 10}
\]

\[
95 \text{CAPF1}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF2}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CAPF3}(I) = \frac{(\text{PH}(I)^2)}{120} - \frac{(\text{PH}(I)^3)}{720}.
\]

\[
\text{CONTINUE}
\]

\[
\text{IS PH BETWEEN ELE2 AND ELE1}
\]

\[
\text{IF(}\text{CONT-1}=101,101,102
\]

\[
102 \text{ CONTINUE}
\]

\[
\text{SPEC}=\text{CI}
\]

\[
\text{GO TO 17}
\]

\[
101 \text{ DO 11 I}=1,\text{N}
\]

\[
104 \text{ IF(ABS(}\text{PH}(I))=\text{ELE1(I))11,11,13
\]

\[
11 \text{ CONTINUE}
\]

\[
12 \text{ SPEC}=\text{CI}
\]

\[
\text{GO TO 15}
\]

\[
\text{HALVE INTERVAL AND DOUBLE PH RANGE}
\]

\[
13 \text{ DO 96 I}=1,\text{N}
\]

\[
96 \text{ CONTINUE}
\]

\[
\text{SPEC}=\text{CI}
\]

\[
\text{GO TO 5}
\]

\[
\text{RETURN TO RECOMPUTE INTERVAL}
\]

\[
\text{RETURN TO RECOMPUTE INTERVAL}
\]

\[
15 \text{ DO 16 I}=1,\text{N}
\]

\[
16 \text{ CONTINUE}
\]

\[
\text{DOUBLE INTERVAL}
\]

\[
165 \text{ CI}=\text{CIMAX}
\]

\[
\text{GO TO 5}
\]

\[
\text{COMPOTE Y4,X4}
\]

\[
\text{DO 18 I}=1,\text{N}
\]

\[
18 \text{ CONTINUE}
\]

\[
\text{CUVAR}(I) = \text{VAR}(I) + \text{SPEC} \times (\text{F3}(I) \times \text{CAPF2}(I) + \text{F1}(I) \times \text{CAPF1}(I) - \text{CAPF2}(I) - \text{CAPF1}(I) - \text{CAPF2}(I))
\]

\[
\text{IF(I.EQ.1) GO TO 18}
\]

\[
\text{IF(CUVA}(R(I))=175,175,18
\]

\[
175 \text{ CI}=\text{SPEC}
\]

\[
\text{CI}=\text{CI}/2.
\]

\[
\text{GO TO 5}
\]

\[
18 \text{ Y4}(I) = \text{CUVAR}(I)
\]

\[
\text{CUVAR}(I) = \text{VAR}(I) + \text{SPEC}
\]

\[
90
\]
APPENDIX A — Continued

CALL BASIC TO EVALUATE F4
CALL BASIC
RETURN
DO 20 I=1,N
11=I+1
F4(1)=DER(1)

C COMPUTE DELTA Y
DELTY(1)=SPEC*(F1(1)*CAPF1(1)+(-3.*(F1(1)+P(1)*VAR(11)))
1+2.*(F2(I)+P(I)+Y2(1)+2.*(F3(1)+P(I)+Y3(I))-F4(I)
2-P(1)*Y4(I))*CAPF2(1)+4.*((F1(I)+P(I)*VAR(I1))-(F2(I)
3+P(1)*Y2(I)-(F3(I)+P(I)+Y3(I))+(F4(I)+P(I)+Y4(I))))*
4CAPF3(I))
C COMPUTE Y+DELTA Y
20 CUVARU1)=VAR(U1)+DELTY(I)
C CALL CHECK FOR DECISION TO ACCEPT OR RECOMPUTE
C INTERVAL
CALL CHECK
IF (ELT121,21,23
C UPDATE Y VALUES
21 N1=N+1
DO 22 I=2,A1
I1=I-1
22 VAR(1)=VAR(I)+DELTY(I1)
VAR(I)=VAR(1)+SPEC
C RETURN TO COMPUTE DERIVATIVES AT Y+DELTA Y
C GO TO 2
C RETURN TO RECOMPUTE INTERVAL
C 23 GO TO 5
C END
APPENDIX A – Continued

The flow charts for the program are presented below:

D1290

1. Initialize
2. Read input
3. Is this a pick-up case?
   - yes: Read tape 13
   - no: Print input
4. CALL SHOCKG to define shock geometry and put on tape 10 x, z, t, R, cos θ, sin θ
5. Compute free-stream quantities
   - M∞, c∞, a∞
6. Compute quantities behind the shock T, e, p, P, u, ¹, ², ³, e, v, i
   - put on tape 11
7. CALL FDPDX to compute p and p put on tapes 9 and 8
8. Initialize for Ψ, streamline KEYINT=0
9. Is estimated time elapsed time < 30 sec?
   - yes: Write data on tape 13 for pickup
   - no: 

(Flow chart details and further steps not fully transcribed due to image quality constraints.)
APPENDIX A - Continued

CALL CALINTH integration routine to update $h, c_i, c_{v,i}$, $i = 1, 1$

BASIC to evaluate derivatives $h, c_j, c_{v,i}$

CALL ITER integrate for $e$

CHECK to test answers

FOFE to evaluate $e$

---

Compute $\sum c_i$

Is any $c_i < 0$?

yes

$NEG = -1$

no

Compute molecular concentration $c_{m,i}$

Print answers

Is $NEG = -1$?

yes

STOP 670

no

Is $IUNEG = 1$?

yes

Extrapolate for $\psi = 0$ values and initialize for $\psi = 0$ streamline

no

Are physical space calculations desired at this $x$?

yes

Save $1/\rho u$ on tape 12

no

Is $x = x_{terminal}$?

yes

no

---

93
APPENDIX A – Continued

Have all ψ values been computed?

Compute and print physical space values

yes

no

END
Evaluate derivatives \( \dot{\epsilon}_i, \dot{\epsilon}_{\nu,i}, \dot{h}_i = 1, 1 \)

Is ITNEG = 1 or IEXP = 1?
- Yes: RETURN
- No:
  - Is \( M = 0 \)?
    - Yes: Put \((e_{\nu,i})_i=1,1\) in proper place in single precision array
    - No: Interpolate for \( p \) & \( \dot{p} \) at \( x \)

Is KEYINT = 1?
- Yes:
  - Is KEYINT = 0?
    - Yes: Compute \( T_{\nu,i}, \nu, u^2 \)
      - Is \( u^2 < 0.0 \)?
        - Yes: IUNEG = -1, RETURN
        - No: Compute \( u \)
          - Compute \( e \)
            - CALL ITRI to iterate for \( e \)
            - FPPF to evaluate \( e \)
        - Make new \( e \) estimate
      - Did \( e \) converge?
        - Yes: STOP
        - No: Has \( e \) been reestimated 2 times?
          - Yes: RETURN
          - No: Compute \( \rho, T \)

Compute \( \rho, T \)
- Is \( T < 0.0 \)?
  - Yes: PRINT "T NEG", E+h*0.000001 x h; ITNEG = 1
  - No: Compute \( \delta \) for each reaction, \( j \) for each species, \( i \), \( \dot{\epsilon}_i, \dot{\epsilon}_{\nu,i}, \dot{h}_i = 1, 1 \)
    - If \( M = 0 \)
      - \( v_{\nu,i} = ?v_{\nu,i} \)
    - Compute \( \delta \)
CHECK

Test answers

Is ITNEG = 0?

yes

Is any c_i < 0?

no

Is \( \frac{T_{prev} - T}{T} < .3 \)?

yes

Is \( \frac{H_{prev} - H}{H} > .01 \)?

no

Is the computing interval < 1.0E-18?

no

Reduce computing interval by 1/4 and recompute

yes

PRINT

STOP 30

RETURN

RETURN
APPENDIX A – Concluded

The deck setup is as follows:

The diagram shows the sequence of cards as follows:

1. EOF card
2. SPECIES & REACTION CARDS
3. END NAMELIST INPUT
4. $NAM1 NAMELIST INPUT
5. CASE ID CARD
6. EOR card
7. DI290 MAIN PROGRAM AND SUBROUTINES
8. EOR card
9. JOB AND CONTROL CARDS
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),

$$
\left[ \frac{\partial c_i}{\partial x} \right]_{\psi_j} = \left[ \frac{K_j \mu_i}{\rho u} \left( \psi'_{1,j} - \nu_{1,j} \right) \right] \sum_{i=1}^{I} \left( \frac{pc_i}{\mu_i} \right)^{\nu_{1,j}} \left( \frac{pc_M}{\mu_M} \right)^{\nu_{I+1,j}}
$$

(\text{B1})


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

$$
c_M = \sum_{i=1}^{I} a_{i,j} c_i
$$

(\text{B2})

and the molecular weight $\mu_M$ is

$$
\mu_M = \sum_{i=1}^{I} m_i \mu_i
$$

(\text{B3})

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

$$
m_i = \frac{p_{M,i}}{p_M}
$$

(\text{B4})

and

$$
p_{M,i} = \frac{c_i \mu}{\mu_i} p_{a_{i,j}}
$$

(\text{B5})

By using Dalton's law of partial pressures

$$
p_M = \sum_{i=1}^{I} p_{M,i}
$$

(\text{B6})
Substituting the three relations (eqs. (A4), (A5), and (A6)) into equation (A3) results in

\[
\mu_M = \frac{\sum_{i=1}^{I} c_i a_{i,j}}{\sum_{i=1}^{I} c_i a_{i,j} \mu_i}
\]  

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

\[
\left[ \frac{\partial c_i}{\partial X_j} \right] = \left[ \frac{K_i \mu_i}{\rho u} \left( \nu_i,j - \nu_{1,j} \right) \right] \prod_{i=1}^{I} \left( \frac{\rho c_i}{\mu_i} \right)^{\nu_i,j} \left( \rho \sum_{i=1}^{I} \frac{c_i a_{i,j}}{\mu_i} \right)^{\nu_i+1,j}
\]  

(B7)
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.

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

The species are \( \text{CO}_2, \text{CO}, \text{CO}^+, \text{C}_2, \text{C}, \text{O}, \text{C}^+, \text{O}^+ \), and \( e^- \) for Case III.

<table>
<thead>
<tr>
<th>Number</th>
<th>Reaction</th>
<th>Rates</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \text{CO}_2 + \text{M} \rightarrow \text{CO} + \text{O} + \text{M} )</td>
<td>( 6.955 \times 10^{12} , T^{1/2} \exp \left( - \frac{63286}{T} \right) )</td>
<td>36</td>
</tr>
<tr>
<td>2</td>
<td>( \text{CO} + \text{O} + \text{M} \rightarrow \text{CO}_2 + \text{M} )</td>
<td>( 3.39 \times 10^6 , T^{1.6175} )</td>
<td>36</td>
</tr>
<tr>
<td>3</td>
<td>( \text{CO} + \text{M} \rightarrow \text{C} + \text{O} + \text{M} )</td>
<td>( 7.72 \times 10^{12} , T^{1/2} \exp \left( - \frac{128925}{T} \right) )</td>
<td>36</td>
</tr>
<tr>
<td>4</td>
<td>( \text{C} + \text{O} + \text{M} \rightarrow \text{CO} + \text{M} )</td>
<td>( 2.26 \times 10^8 , T^{0.7366} \exp \left( \frac{665}{T} \right) )</td>
<td>36</td>
</tr>
<tr>
<td>5</td>
<td>( \text{C} + \text{O} \rightarrow \text{CO}^+ + e^- )</td>
<td>( 2.049 \times 10^{12} \exp \left( - \frac{33300}{T} \right) )</td>
<td>40</td>
</tr>
<tr>
<td>6</td>
<td>( \text{CO}^+ + e^- \rightarrow \text{C} + \text{O} )</td>
<td>( 6.023 \times 10^{16} )</td>
<td>40</td>
</tr>
<tr>
<td>7</td>
<td>( \text{C} + e^- \rightarrow \text{C}^+ + 2e^- )</td>
<td>( 2.09 \times 10^{14} , T^{0.5} \exp \left( - \frac{130713}{T} \right) )</td>
<td>41</td>
</tr>
<tr>
<td>8</td>
<td>( \text{C}^+ + 2e^- \rightarrow \text{C} + e^- )</td>
<td>( 9.65 \times 10^{21} , T^{-0.836} )</td>
<td>41</td>
</tr>
<tr>
<td>9</td>
<td>( \text{O} + e^- \rightarrow \text{O}^+ + 2e^- )</td>
<td>( 2.14 \times 10^{14} , T^{0.5} \exp \left( - \frac{158000}{T} \right) )</td>
<td>41</td>
</tr>
<tr>
<td>10</td>
<td>( \text{O}^+ + 2e^- \rightarrow \text{O} + e^- )</td>
<td>( 6.05 \times 10^{22} , T^{-2} )</td>
<td>41</td>
</tr>
<tr>
<td>11</td>
<td>( \text{C}_2 + \text{M} \rightarrow 2\text{C} + \text{M} )</td>
<td>( 6.74 \times 10^{13} , T^{0.5} \exp \left( - \frac{70529}{T} \right) )</td>
<td>41</td>
</tr>
<tr>
<td>12</td>
<td>( 2\text{C} + \text{M} \rightarrow \text{C}_2 + \text{M} )</td>
<td>( 1.61 \times 10^{12} , T^{0.743} )</td>
<td>41</td>
</tr>
</tbody>
</table>
APPENDIX C – Concluded

Cases IV and V

The species are CO₂, CO, C, O, A, C⁺, A⁺, and e⁻ for Cases IV and V.

<table>
<thead>
<tr>
<th>Number</th>
<th>Reaction</th>
<th>Rates</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CO₂ + M → CO + O + M</td>
<td>$6.955 \times 10^{12} \ T^{1/2} \exp\left(-\frac{63.286}{T}\right)$</td>
<td>36</td>
</tr>
<tr>
<td>2</td>
<td>CO + O + M → CO₂ + M</td>
<td>$3.39 \times 10^6 \ T^{1.6175}$</td>
<td>36</td>
</tr>
<tr>
<td>3</td>
<td>CO + M → C + O + M</td>
<td>$7.72 \times 10^{12} \ T^{1/2} \exp\left(-\frac{128.925}{T}\right)$</td>
<td>36</td>
</tr>
<tr>
<td>4</td>
<td>C + O + M → CO + M</td>
<td>$2.26 \times 10^8 \ T^{0.7366} \exp\left(\frac{665}{T}\right)$</td>
<td>36</td>
</tr>
<tr>
<td>5</td>
<td>C + e⁻ → C⁺ + 2e⁻</td>
<td>$2.09 \times 10^{14} \ T^{0.5} \exp\left(-\frac{130.713}{T}\right)$</td>
<td>41</td>
</tr>
<tr>
<td>6</td>
<td>C⁺ + 2e⁻ → C + e⁻</td>
<td>$9.65 \times 10^{21} \ T^{-0.836}$</td>
<td>41</td>
</tr>
<tr>
<td>7</td>
<td>O + e⁻ → O⁺ + 2e⁻</td>
<td>$2.14 \times 10^{14} \ T^{0.5} \exp\left(-\frac{158}{T}\right)$</td>
<td>41</td>
</tr>
<tr>
<td>8</td>
<td>O⁺ + 2e⁻ → O + e⁻</td>
<td>$6.05 \times 10^{22} \ T^{-2}$</td>
<td>41</td>
</tr>
<tr>
<td>9</td>
<td>C + O → CO⁺ + e⁻</td>
<td>$2.049 \times 10^{12} \exp\left(-\frac{33.300}{T}\right)$</td>
<td>40</td>
</tr>
<tr>
<td>10</td>
<td>CO⁺ + e⁻ → C + O</td>
<td>$6.023 \times 10^{16}$</td>
<td>40</td>
</tr>
<tr>
<td>11</td>
<td>A + e⁻ → A⁺ + 2e⁻</td>
<td>$1.94 \times 10^{14} \ T^{0.5} \exp\left(-\frac{182.830}{T}\right)$</td>
<td>41</td>
</tr>
<tr>
<td>12</td>
<td>A⁺ + 2e⁻ → A + e⁻</td>
<td>$8.55 \times 10^{21} \ T^{-1.075}$</td>
<td>41</td>
</tr>
</tbody>
</table>
REFERENCES


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

(b) Nitrogen atom.

\[ \frac{x - x_s}{R_{c,0}} \]

Figure 6.—Continued.
Figure 6.- Continued.

\[ \frac{x - x_s}{R_{c,0}} \]

(c) NO.
Ref. 8
Present method

(d) Electron.

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(a) Oxygen atom.
(b) Nitrogen atom.

Figure 10.- Continued.
Figure 10.- Continued.
(d) Electron.

Figure 10.—Concluded.
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\[ z_s = \frac{r_s^2}{1 + 1.732 \ r_s} \]
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\[ \tilde{x} = \tilde{x}_s \]

(a) \( \tilde{x} = 0.5; O, CO, C, CO_2. \)
Figure 19.- Continued.

(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) $\mathcal{K} = 0.5; C_2$.

Figure 19.- Continued.
Figure 19.— Concluded.

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Figure 19.— Concluded.
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(c) C, CO⁺, and e⁻.
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\[ z_s = \frac{r_s^2}{1 + 1.98 r_s} \]

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(a) A, CO, O, and CO$_2$.

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

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