FINITE-RATE CHEMISTRY EFFECTS UPON CONVECTIVE AND RADIATIVE HEATING OF AN ATMOSPHERIC ENTRY VEHICLE

by

Guillermo Perez

under the direction of

Richard C. Farmer

&

Ralph W. Pike

Prepared Under

Grant NGR 19-001-059

by

Department of Chemical Engineering
Louisiana State University
Baton Rouge, Louisiana 70803

for

Langley Research Center
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This report gives the results for a finite-rate, stagnation-line analysis of the radiative heating of a phenolic-nylon ablator. The analysis includes flowfield coupling with the ablator surface, binary diffusion, and a coupled line and continuum radiation model. This report serves as a user's manual and operating instructions for the computer programs listed in this document. This analysis has been incorporated into an around-the-body analysis by these same principal investigators. Copies of the decks which are used to accomplish this later analysis have been supplied to Dr. James N. Moss, grant monitor, of the NASA, Langley Research Center.

This report also served as Guillermo Perez's dissertation requirement in obtaining a Doctor of Philosophy degree in Chemical Engineering.
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NOMENCLATURE

English

$B_v$ Planckian radiation intensity (m/t² x no. of particles)

$C_i$ Mass fraction (mass of i/unit mass of fluid)

\[ C_i = \frac{\rho_i}{\rho}, \quad \sum_i C_i = 1 \]

$C_p$ Specific heat at constant pressure (L²/t² x T)

$C_{pi}$ Species specific heat at constant pressure

\[ (L²/t² x T x \text{mole of } i) \]

$D$ Diffusion coefficient (L²/t)

$D_T$ Thermal diffusion coefficient (m/L x t)

$D_{ij}$ Binary diffusion coefficient (L²/t)

$\mathcal{E}$ Radiative flux divergence (m/L x t²)

$f$ Velocity function defined by Eq. 4.14

$f_j$ Forward reaction rate constant for the jth reaction

$F$ Gibbs free energy (mL²/t²)

$F_i$ Species Gibbs free energy (mL²/t² x mole of i)

$H$ Total enthalpy, \( H = h + \frac{u^2}{2} \) (L²/t²)

$h$ Static enthalpy, \( h = Q + P/\rho \) (L²/t²), also Planck's constant

$h_i$ Species static enthalpy (L²/t² x mole of i)

$I_v$ Spectral radiation intensity (m/t² x no. of particles)
\( J_{iy} \) Mass diffusion component for the \( i \)th species in a direction normal to the body surface \((m/L^2 \times t)\)

\( k \) Coefficient of thermal conductivity \((mL/t^3 \times T)\)

\( K_j \) Equilibrium constant for the \( j \)th reaction

\( M_i \) Molecular weight of species \( i \) \((\text{mass of } i/\text{mole of } i)\)

\( m \) Number of chemical reactions occurring in the flow-field

\( m_i \) Mass of \( i \) \((m)\)

\( N \) Number density \((\text{particles}/L^3)\)

\( n \) Number of chemical species present in the flow-field

\( n_i \) Species molal density \((\text{moles of } i/L^3)\)

\( P \) Static pressure \((m/L \times t^2)\) or \((F/L^2)\)

\( Q \) Internal energy per unit mass, including chemical energy \((L^2/t^2)\), also total energy flux to a surface \((m/t^3)\)

\( q_{R,y} \) Radiative heat flux component in a direction normal to the body surface \((m/t^3)\) or \((E/L^2 \times t)\)

\( Q_c \) Convective energy flux to a surface \((m/t^3)\)

\( Q_D \) Diffusive energy flux to a surface \((m/t^3)\)

\( Q_R \) Radiative energy flux to a surface \((m/t^3)\)

\( R \) Body nose radius \((L)\)

\( R_e \) Reynolds number \( \rho \infty U \rho \sqrt{R/\mu} \)
<table>
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<th>Symbol</th>
<th>Term</th>
<th>Definition</th>
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<td>Re₈</td>
<td>Reynolds number</td>
<td>$\rho_{s, o} U_\infty R/\mu_{s, o}$</td>
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<tr>
<td>IR</td>
<td>Universal gas constant</td>
<td>$(mL^3/t^2 \times T \times \text{no. of moles})$</td>
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<tr>
<td>r</td>
<td>Cylindrical body radius</td>
<td>defined in Fig. 2.1 (L)</td>
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<td>r_j</td>
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<td>S</td>
<td>Entropy</td>
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<td>S_i</td>
<td>Species entropy</td>
<td>$(L^2/t^2 \times T \times \text{mole of } i)$</td>
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<td>T</td>
<td>Thermodynamic temperature</td>
<td>(T)</td>
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<tr>
<td>t</td>
<td>Time</td>
<td>(t)</td>
</tr>
<tr>
<td>U_∞</td>
<td>Freestream velocity</td>
<td>$(L/t)$</td>
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<tr>
<td>u</td>
<td>Velocity component in a direction parallel to the body surface</td>
<td>$(L/t)$</td>
</tr>
<tr>
<td>v</td>
<td>Velocity component in a direction normal to the body surface</td>
<td>$(L/t)$ also frequency $(l/t)$</td>
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<tr>
<td>x</td>
<td>Body oriented coordinate</td>
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<td>y</td>
<td>Body oriented coordinate</td>
<td>defined in Fig. 2.1</td>
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<tr>
<td>y_i</td>
<td>Mole fraction of species i</td>
<td>$\sum y_i = 1$</td>
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<tr>
<td>(\alpha_g)</td>
<td>Volumetric absorption coefficient, effective</td>
<td>$(L^2 \times \text{no. of particles}/L^3)$</td>
</tr>
<tr>
<td>(\delta)</td>
<td>Shock detachment distance</td>
<td>(L)</td>
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<td>(x_i)</td>
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\( \delta \) Transformed shock detachment distance

\( \varepsilon \) Difference between the body and shock angle \( \varepsilon = \theta - \phi \) radians

\( \eta \) Dorodnitzyn variable

\( \theta \) Body angle (radians)

\( \kappa \) Local body curvature (1/L)

\( \kappa \) \( 1 + \gamma \)

\( \Lambda \) Diffusional or radiative flux divergence (see Eq. 2.12) \( (\text{m}/\text{L} \times \text{t}^2) \)

\( \lambda \) \( (\mu - 2/3 \mu) \) \( (\text{m}/\text{L} \times \text{t}) \)

\( \mu \) Ordinary viscosity \( (\text{m}/\text{L} \times \text{t}) \)

\( \mu \) Bulk viscosity \( (\text{m}/\text{L} \times \text{t}) \)

\( \nu \) Frequency \( (\text{l}/\text{t}) \)

\( \xi \) Nondimensional x-coordinate

\( \rho \) Density \( (\text{m}/\text{L}^3) \)

\( \rho_i \) Partial density of species \( i \), \( \rho_i = n_i M_i \) \( (\text{m of } i/\text{L}^3) \)

\( \varphi \) Density ratio across shock

\( \phi \) Shock angle (radians)

\( \omega_i \) Generation of species \( i \) \( (\text{m}/\text{L}^3 \times \text{t}) \)
Subscripts

D  Diffusion

e  Edge conditions

i  Species i

n  Normal component

r  Radiation

T  Tangential component or total quantity

v  Spectral

w  Wall quantities

x  Component in a direction parallel to the body surface

y  Component in a direction normal to the body surface

oo  Freesream conditions

s, δ  Quantities immediately behind the shock

Superscripts

A  0 or 1 denoting two-dimensional or axisymetric respectively (an exponent)

T  Thermal

*  Denotes dimensional variables

0  Standard state quantity

-  Evaluated on char side of ablator interface

+  Evaluated on flow-field side of ablator interface

** Symbols not listed are defined where used.

$ Abbreviations mean: m, mass; L, length; t, time; T, temperature; F, force; E, energy
ABSTRACT

A mathematical model of the aerothermochemical environment along the stagnation line of a planetary return spacecraft using an ablative thermal protection system was developed and solved for conditions typical of atmospheric entry from planetary missions. The model, implemented as a Fortran IV computer program, was designed to predict viscous, reactive and radiative coupled shock layer structure and the resulting body heating rates. The analysis includes flow-field coupling with the ablator surface, binary diffusion, coupled line and continuum radiative and equilibrium or finite-rate chemistry effects. The gas model used includes thermodynamic, transport, kinetic and radiative properties of air and ablation product species, including 19 chemical species and 16 chemical reactions. Specifically, the impact of non-equilibrium chemistry effects upon stagnation line shock layer structure and body heating rates was investigated.

The mathematical model forms a set of twenty-six algebraic, differential and integrodifferential non-linear equations subject to two-point boundary conditions. The numerical solution was carried out by decoupling, linearizing and finite differencing the equations in a iterative, globally-implicit manner.

The model was used to determine the finite-rate chemistry and chemical-equilibrium stagnation line heating rate of a 9 foot entry vehicle protected by a phenolic-nylon ablator and moving at 50,000 feet/second when the free-stream air density is $8.85 \times 10^{-8}$ slugs/ft$^3$ and the mass injection rate equals .05. The results obtained predict significantly different shock layer properties for the finite-rate
case and for the chemical equilibrium case. The ablation products entering the shock layer through the body wall react much slower than under equilibrium conditions and the air components entering the shock layer through the shock are not de-ionized, as predicted by the equilibrium analysis, but remain "frozen" throughout most of the shock region. The total heating rate to the body was found to be significantly lower under non-equilibrium than under equilibrium chemistry conditions. This difference was attributed to lower concentrations of optically active species, such as N and O, over most of the shock layer in the non-equilibrium chemistry case.

On the basis of this research it was concluded that a finite-rate stagnation-line shock layer solution which contains a reasonable kinetics model to describe atmospheric entries protected by phenolic-nylon ablators was successfully developed. It was also concluded that, for the flight conditions considered, finite-rate chemistry effects are significant since both shock layer structure and body heating rates are markedly different from those predicted by chemical equilibrium analyses.

It was recommended that additional studies be carried out on: 1.) improving the computational speed of the solution; 2.) finite-rate chemistry effects under flight conditions different from those considered in this work; 3.) the effect of assuming more realistic shock and wall boundary conditions; and 4.) determining solutions for coupled non-equilibrium ablator response and shock layers. The computational speed of the solution should be improved so that SLAC is developed from a research program to an effective engineering tool. Studies of finite-rate chemistry effects under flight conditions different from those considered here should be carried out to determine the range of
conditions over which solutions may be obtained using the implemented model, and the range of conditions over which non-equilibrium chemistry effects are significant and how they affect the body heating rates. The boundary conditions studies should investigate the possible non-equilibrium composition of air, including detailed studies of the pertinent kinetics at the shock, (in the present work the chemical equilibrium composition was used), and the use of boundary conditions of the third kind at the wall. Coupled solutions for both non-equilibrium ablator behavior and shock layers should be determined to obtain a complete solution to the quasi-steady entry problem.
CHAPTER 1
INTRODUCTION

THE NATURE OF THE REENTRY PROBLEM

The launching of a suborbital, orbital or superorbital flight requires that some means of propulsion be utilized to propel the spacecraft against the force of gravity. In practice, a chemically-fueled rocket engine is used. The increase in the speed of the spacecraft results in an increase in its kinetic energy while its motion through the gravitational force field results in an increase in its potential energy. This kinetic and potential energy would be converted into the same amount of kinetic energy if the spacecraft were allowed to fall freely towards the Earth and there was no atmosphere. This would result in fantastic landing speeds and the destruction of the spacecraft upon its collision with the surface of the Earth. Obviously, additional propulsive power would have to be used in a direction opposite to the force of gravity in order to decelerate the spacecraft until reasonable landing speeds are obtained. This need for additional propulsive power results in a decrease of the payload since some of the weight of the spacecraft has to be used for the propulsion hardware. N.A.S.A.'s Moon landings are accomplished precisely in this manner.

Deceleration of entry vehicles can be accomplished by: 1) use of propulsive power against the pull of gravity, and 2) use of aerodynamic drag. Landing of spacecrafts on celestial bodies lacking an atmosphere
precludes the use of the second technique. Aerodynamic braking requires transfer of the body's kinetic and potential energy to the atmosphere and results in the heating of the air in the vicinity of the body. Part of the energy gained by the air is then transferred to the body by convection and radiation creating a need for thermal protection of the spacecraft. Both the propulsive and aerodynamic drag braking techniques require a reduction of the payload since in the former the propulsion hardware and in the latter the heat shield must be a part of the spacecraft. The optimum technique to be used varies with mission characteristics and should be chosen according to a number of factors, such as the level of heat shielding technology and payload. Less payload penalty is suffered by using aerodynamic braking than propulsive braking for braking from hyperbolic approach velocities to orbital velocities at Mars (Ref. 1.1).

**DESCRIPTION OF THE FLOW-FIELD IN THE VICINITY OF THE BODY**

Of primary importance, in establishing entry heating levels, is the magnitude of the speeds that will be encountered. The range of Earth entry speeds associated with several mission objectives is given in Figure 1.1 (Ref. 1.2). The use of the gravitational field of Venus to alter the interplanetary trajectories between Mars and Earth (Venus swingby) is shown to result in significantly reduced Earth entry speeds when compared to direct trajectories. Of particular interest are entry speeds of about 50,000 fps (about 15 km/sec) since the capability of entering at these speeds will permit a wide variety of trips to Mars, Venus and the asteroids.

A blunt body of the type used by NASA in its manned spacecraft program (Figure 1.2) would show, under conditions prevalent during atmospheric entry at speeds of approximately 50,000 fps, a standing bow
Figure 1.1 Earth Entry Speeds for Several Mission Objectives
(From Ref. 1.2)
Figure 1.2 Flow-Field in the Vicinity of a Blunt Body
shock due to the deceleration of the air in the vicinity of the body. The blunt body of Figure 1.2 is axisymmetric and is shown flying at a zero angle of attack (its axis of symmetry coincides with the translational vector), this means that the shock and the flow field between the shock and the body are axisymmetric. The region of the flow field between the shock and the surface of the body may be divided into the stagnation line, so-called because the velocity is zero somewhere along this line, and the around-the-body region. When the body wall is impermeable, the stagnation point is at the wall where both the normal and tangential components of velocity are zero.

It is important to note, that even though viscous effects are in part responsible for the generation of the high temperatures present, they are not solely responsible since even for inviscid fluids there would be a deceleration of the fluid at the stagnation line. Thus the difference between viscous and inviscid flow fields would not be basic in nature.

THERMAL PROTECTION SYSTEMS

The task of protecting the vehicle from the heat generated during atmospheric entry may be accomplished in a number of ways: use of heat sinks, transpiration cooling, radiation cooling, ablative cooling, etc. The use of a heat sink as a thermal protection system is very limited by the lack of suitable materials with high heat capacity and low thermal conductivity. Transpiration cooling involves the injection of a cool fluid into the shock layer so that it absorbs heat and insulates the vehicle from the high temperatures. Radiation cooling involves the use of a highly reflective structure in order to block the transfer of radiative heat into the body. Ablative heat shields operate with materials that undergo endothermic physical and chemical changes.
Of all the methods of thermal protection, ablative cooling has been the most successful. This type of thermal protection system may be either a non-charring or a charring ablator. The former type of ablator is one that changes from a solid to a gaseous state and enters the shock layer counter to the heat flow; typical of these materials is Teflon. Charring ablators, on the other hand, decompose to a porous char and relatively low molecular weight gases. The latter type ablator has enjoyed widespread use in the space program.

The principal thermal protection mechanisms in a charring ablator are shown in Figure 1.3. Blockage occurs when the pyrolysis gases are injected into the shock layer and prevent most of the convective heat flux from reaching the body surface. The ablation products in the shock layer absorb part of the radiative flux from the shock and also react endothermically. Char re-radiation stops part of the radiative flux to the body while, if the temperature is high enough, sublimation of the char absorbs part of the incoming energy. The further "cracking" of pyrolysis gases and the process of heating those gases from the temperature at the decomposition zone to the shock layer temperature and their subsequent injection into the shock layer constitute additional protection mechanisms. The decomposition process in the pyrolysis zone which initially produces the pyrolysis gas also absorbs heat. Finally, any heat not absorbed elsewhere may be stored in the virgin material in which case the process acts as a simple heat sink.

THE NEED FOR A BETTER UNDERSTANDING OF THE AERODYNAMIC BRAKING PROCESS

Results from a study of the possible effects of uncertainties in analyses upon heat shield weight are given in Fig. 1.4 (Ref. 1.2). The factors considered were uncertainties in: air absorption coefficients,
Figure 1.3 Thermal Protection Mechanisms (From Ref. 1.2)
Figure 1.4 Results of Uncertainty Analysis for an Entry Speed of 15 km/sec
(From Ref. 1.2)
boundary layer transition, transpiration effectiveness, surface emissivity, char sublimation, and pyrolysis gas enthalpy. The entry speed considered is 50,000 fps and the weights are normalized to those for the nominal conditions as shown at the top. Results for each perturbation are stated. It should be noted that the only perturbation causing a decrease in heat shield weight is the surface emissivity. Since the effect of some of the uncertainties can be additive it is evident that a weight increase of 50 percent or more is possible. For the range of entry speeds of interest in this study the heat shield is estimated to represent between 10 and 20 percent of the entry-vehicle weight. Due to the uncertainties mentioned above this value can represent as high as 15 to 30 percent of the entry vehicle weight with a corresponding reduction in the payload returnable to Earth. Such an effect is clearly not negligible.

One obvious way of reducing these uncertainties is by experimental verification of the thermal environment about the spacecraft. Such a verification requires duplication of a number of parameters like: flight velocity, free-stream density, enthalpy and flow energy, etc. Unfortunately, the presently existing ground testing facilities are not capable of simultaneous duplication of all the important parameters (Refs. 1.2, 1.4). The alternatives to ground testing are: testing under actual flight conditions or developing accurate mathematical models to describe the aerodynamic braking process. Because of the very high costs involved in flight testing, the importance of improving existing analytic models is evident.

The pyrolysis gas enthalpy uncertainty, being the largest has since being studied (Ref. 1.4). For entry speeds greater than 50,000
fps, the effect of the radiation heat transfer uncertainty should become increasingly important since at these higher speeds the ratio of heat transfer by radiation to heat transfer by convection increases. A recent study by Engel (Ref. 1.5) resulted in development of a model that includes line and continuum radiation and equilibrium chemistry with no diffusion. Each (Ref. 1.6) used the same radiation model used by Engel and obtained solutions for binary and multicomponent diffusion of gas mixtures in chemical equilibrium.

Radiative properties are dependent, among other things, upon chemical composition. For this reason it is important to use the correct chemical model when computing heating rates. The chemical equilibrium assumption greatly simplifies the problem since it eliminates the need for consideration of chemical kinetics. When conditions in the flowfield are such that the actual chemical composition is close to the chemical equilibrium composition, then the use of an equilibrium model is valid. This generally occurs when the pressure and temperature are high. On the other hand for low pressures and temperatures the difference between the actual and equilibrium compositions may be large and a finite-rate chemistry model must be used.

**STATEMENT OF OBJECTIVES**

This study was undertaken in an effort to reduce uncertainties in reentry heating resulting from non-equilibrium chemistry effects. The state-of-the art upon which improvements will be made is given in Refs. 1.5 and 1.6. Specifically, the current research will try to fulfill the following objectives:

1. Develop and solve a mathematical model of the flow-field along the stagnation-line of the shock layer. The model shall
include the effects of line and continuum radiation, thermodynamic and transport properties of air and ablation products, binary diffusion, and finite-rate chemistry.

2. Determine whether finite-rate chemistry effects significantly change the heating rate from the one obtained by assuming the flow is in chemical equilibrium.

REFERENCES


1.5 Engel, Carl D., Ablation and Radiation Coupled Viscous Hypersonic Shock Layers, Ph.D. Dissertation, Louisiana State University, Baton Rouge, Louisiana (1971)

1.6 Esch, Donald D., Stagnation Region Heating of a Phenolic-Nylon Ablator During Return from Planetary Missions, Ph.D. Dissertation, Louisiana State University, Baton Rouge, Louisiana (1971).
CHAPTER 2

DEVELOPMENT OF THE FLOW-FIELD EQUATIONS

The mathematical model which describes the flow-field at the stagnation line is developed in this chapter. The conservation equations for the flow-field between the body and the shock with the appropriate wall and shock boundary conditions are developed. From these equations, the stagnation line conservation equations and boundary conditions are derived.

CONSERVATION EQUATIONS OF THE SHOCK LAYER

The mathematical model of the flowfield from the body surface to the shock is obtained from the laws of conservation of mass, momentum and energy and also from the formulation of a gas model. The gas model used will be discussed in the latter part of this chapter as well as in Chapter 3. The complete body oriented conservation equations for a multicomponent, viscous, radiating, chemically reacting fluid at steady state were developed by Engel (Ref. 2.1). The body oriented coordinate system and shock layer geometrical relations pertinent to these conservation equations are given in Figure 2.1.

However, these equations are far too complex to allow solution with presently available techniques. Fortunately, it has been found that, in general, solution of the complete conservation equations is not necessary since some of the terms in the equations do not significantly contribute to the solution and may therefore be neglected. Of
\[ \tan \epsilon = \frac{d\delta}{(1 + \kappa \delta) dx} \quad \frac{d\theta}{dx} = \kappa(x) \]

\[ \delta = \int_{\gamma} (1 + \kappa \delta) \tan \epsilon \, dx + \delta_0 \quad \theta = \int_{\gamma} \kappa(x) \, dx \]

Figure 2.1 Body-Oriented Coordinate System
course, which terms, if any, are negligible varies with flow conditions and must be determined in each particular case. It will be shown below that, for the flight conditions of interest, the shock layer is laminar, thin is a continuum and these facts can be used to obtain the order of magnitude of the terms in the conservation equation.

According to the results of Hayes and Probstein (Ref. 2.2) the gas behind a bow shock of a hypervelocity vehicle is a continuum when the free-stream Reynolds number (Re) satisfies the relation

\[ Re = \frac{\rho_{\infty} U_{\infty} R}{\mu_{\delta,0}} > 100 \]  

(2.1)

Further, for free-stream Reynolds numbers greater than 100, the standoff distance divided by body radius \((\delta*/R*)\) has been shown to be approximately equal to the ratio of the pre-shock density \((\rho_*)\) to the post-shock density \((\rho_{\delta}^*)\) (Ref. 2.2).

\[ \frac{\delta^*}{R^*} = \frac{\rho_{\infty}}{\rho_{\delta}^*} = \rho \]  

(2.2)

Finally, for hypersonic Mach numbers the density ratio across the shock \((\rho)\) is of the order of one tenth and less for dissociating gases.

\[ \rho \leq 0.10 \]  

(2.3)

An estimate of the dimensionless standoff distance can be obtained from Eqs. 2.1 and 2.2.

\[ \frac{\delta^*}{R^*} \leq 0.10 \]  

(2.4)

In this chapter a superscript * will denote dimensional variables unless it is explicitly stated otherwise.
Since the dimensionless distance in a direction parallel to the body \((X^*/R^*)\) is of order 1 and greater while the dimensionless distance in a direction normal to the body is of order \(\frac{1}{10}\) and less, this means that the shock layer is thin.

In order to determine the order of magnitude of the terms in the conservation equations following the methods of Ref. 2.3, the equations are nondimensionalized by using constants characteristic of the flow field, for example

\[
\begin{align*}
\xi &= \frac{X^*}{R^*} \\
y &= \frac{Y^*}{R^*} \\
u &= \frac{u^*}{U_{\infty}^*} \\
v &= \frac{v^*}{U_{\infty}^*}
\end{align*}
\] (2.5)

The order of magnitude of the dependent and independent variables is determined by using the largest possible magnitude of the dimensional variable, for example,

\[
\begin{align*}
\xi \frac{R^*}{R^*} &= 1 \\
y \frac{\delta^*}{R^*} &= \frac{\rho}{\rho} \\
u \frac{U_{\infty}^*}{U_{\infty}^*} &= 1
\end{align*}
\] (2.6)

Using the above procedure, the orders of magnitude of the terms in the conservation equations were determined (Ref. 2.1) and are given in Table 2.1. All terms of order \(\rho^{-2}\) and higher have been dropped from all equations except the y-momentum equation. The dimensionless variables appearing in Eqs. 2.7 - 2.12 are defined in Table 2.2. It must be noted that Eqs. 2.8, 2.9 and 2.10 contain terms of unknown order of magnitude.
TABLE 2.1
LISTING OF CONSERVATION EQUATION WITH
ORDER ASSESSMENT RESULTS

Global continuity:

\[
0[1] \quad 0[1] \\
\frac{\partial}{\partial \xi} (r^A \rho u) + \frac{\partial}{\partial y} (\tilde{\nu} r^A \rho v) = 0 \quad (2.7)
\]

Species continuity:

\[
0[1] \quad 0[1] \quad 0[1] \\
\frac{\partial}{\partial \xi} (r^A \rho C_i u) + \frac{\partial}{\partial y} (\tilde{\nu} r^A \rho C_i v) = - \frac{\partial}{\partial y} (\tilde{\nu} r^A J_{1y}) + \tilde{\nu} r^A \omega_i \quad (2.8)
\]

\(\xi\) - momentum:

\[
0[1] \quad 0[1] \quad 0[\rho] \\
\rho r^A u \frac{\partial u}{\partial \xi} + \rho r^A v \frac{\partial u}{\partial y} + \rho r^A u v + r^A \frac{\partial P}{\partial \xi} \\
0\left[ \frac{1}{\rho} \right] \quad 0\left[ \frac{1}{\rho} \right] \quad 0\left[ \frac{1}{\rho} \right] \quad (2.9)
\]

\[ - \frac{1}{Re} \left\{ \frac{\partial}{\partial y} (\tilde{\nu} r^A \mu \frac{\partial u}{\partial y}) - \frac{\partial}{\partial y} (\tilde{\nu} r^A \mu) + \tilde{\nu} r^A \mu \frac{\partial u}{\partial y} \right\} = 0 \]
TABLE 2.1 (Cont.)

$y$ - momentum: ( $0[\rho]$ and larger terms)

\[\begin{align*}
0[\rho] & \quad 0[\rho] & 0[1] \\
\rho r_A^2 \frac{\partial v}{\partial y} + \rho r_A^2 \frac{\partial v}{\partial y} - \rho r_A^2 u \frac{\partial \rho}{\partial y} & \quad 0\left[\frac{1}{\rho}\right] & 0\left[\frac{1}{\rho}\right] \\
- \frac{1}{R_e} \left\{ \frac{\partial}{\partial \xi} \left( r_A^2 \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial}{\partial \xi} (r_A u) \right) \right\} & = 0
\end{align*}\]

$y$ - momentum: ( $0[\rho^{-2}]$ and larger terms)

\[\begin{align*}
0[\rho] & \quad 0[\rho] & 0[1] \\
\rho r_A^2 \frac{\partial v}{\partial y} - \rho r_A^2 \frac{\partial v}{\partial y} - \rho r_A^2 u \frac{\partial \rho}{\partial y} & \quad 0\left[\frac{1}{\rho}\right] & 0\left[\frac{1}{\rho}\right] \\
- \frac{1}{R_e} \left\{ \frac{\partial}{\partial \xi} \left( r_A^2 \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial}{\partial \xi} (r_A u) \right) \right\} & = 0
\end{align*}\]
TABLE 2.1 (Cont.)

Energy:

\[
0[1] \quad 0[1] \quad 0[1] \quad 0[1]
\]

\[
A \frac{\rho u}{\partial \gamma} + \kappa A \frac{\rho v}{\partial \gamma} = -2\Lambda_{D,y} + \Lambda_{R,y}
\]

\[
0\left[ \frac{1}{\rho^2} \right] \quad 0\left[ \frac{1}{\rho^2} \right] \quad (2.12)
\]

\[
+ \frac{2}{R_e} \left\{ \frac{\partial}{\partial y} \left( \kappa A \frac{\rho u}{\partial \gamma} \right) - \frac{\partial}{\partial y} \left( \kappa A \frac{\rho u^2}{\partial \gamma} \right) \right\}
\]
TABLE 2.2
DEFINITION OF DIMENSIONLESS VARIABLES

\[ g = \frac{x^*}{R^*} \quad y = \frac{y^*}{R^*} \quad u = \frac{u^*}{U_{\infty}^*} \quad v = \frac{v^*}{U_{\infty}^*} \]

\[ \rho = \frac{\rho^*}{\rho_{\infty}}, \quad \mu = \frac{\mu^*}{\mu_{s,0}}, \quad \lambda = \frac{\lambda^*}{\mu_{s,0}}, \quad \delta = \frac{\delta^*}{R^*} \]

\[ r = \frac{r^*}{R^*} \quad \kappa = \kappa^* R^* \quad \rho = \frac{P^*}{\rho_{\infty}^*(U_{\infty}^*)^2} \quad h = \frac{H^*}{H_{\infty}^*} \]

\[ h = \frac{h^*}{H_{\infty}^*} \quad \text{where} \quad H^* = \frac{1}{2}U_{\infty}^2 \]

\[ \tilde{\kappa} = 1 + \kappa y \quad w_{\perp} = \frac{R^* w_{\perp}^*}{\rho_{\infty}^*(U_{\infty}^*)} \quad J = \frac{J^*}{\rho_{\infty}^*(U_{\infty}^*)} \quad \Lambda_{R,x} = \frac{A_{R,x}^*}{\rho_{\infty}^*(U_{\infty}^*)^3} \]

\[ \Lambda_{R,y} = \frac{A_{R,y}^*}{\rho_{\infty}^*(U_{\infty}^*)^3} \quad \Lambda_{D,x} = \frac{A_{D,x}^*}{\rho_{\infty}^*(U_{\infty}^*)^3} \quad \Lambda_{D,y} = \frac{A_{D,y}^*}{\rho_{\infty}^*(U_{\infty}^*)^3} \]

where

\[ A_{R,x}^* = \frac{\partial}{\partial x^*}(r^* A_{q_R}^*, x) \quad A_{R,y}^* = \frac{\partial}{\partial y^*}(r^* A_{q_R}^*, y) \]

\[ A_{D,x}^* = \frac{\partial}{\partial x^*}(r^* A_{q_D}^*, x) \quad A_{D,y}^* = \frac{\partial}{\partial y^*}(r^* A_{q_D}^*, y) \]
This means that these terms can not be dropped from the equations since they may or may not be significant.

Two additional assumptions were made in order to simplify the equations of the flow-field. The first of these consists of assuming that Stokes' Postulate (Ref. 2.3) is valid throughout the flow-field. This yields

\[ \mu^* = \frac{2}{3} \mu^* \]  

(2.13)

and simplifies Eqs. 2.10 and 2.11. The radiative energy term in Eq. 2.12 was simplified by assuming that the shock layer geometry is approximated locally by an infinite plane slab in which radiative transport properties vary only across the slab. This assumption yields

\[ \Lambda \left( \frac{\partial}{\partial y} \right) = \frac{\partial}{\partial y} \int_0^\infty \alpha (2B_v - I_v) \, dv \]  

(2.14)

As a result of the bulk viscosity assumption and the planar radiative transfer model Eqs. 2.7-2.12 may be written in a more usable form. The resulting equations are known as the thin shock layer equations and are given in Table 2.3. These equations are also referred to as the second order boundary layer equations with curvature effects.

If all the terms of order \( \nu \) or higher are dropped from the conservation equations they are then known as the first order shock layer equations or the first order boundary layer equations (Table 2.4).

The first order boundary layer equations (Table 2.4) were chosen to describe the flowfield for the following reasons: (1) the Reynolds numbers encountered during Earth atmospheric reentry from typical Mars
TABLE 2.3
SECOND ORDER SHOCK LAYER EQUATIONS

Global continuity:

\[ \frac{\partial}{\partial x} (\text{r}^A \rho u) + \frac{\partial}{\partial y} (\text{r}^A \rho v) = 0 \]  \hspace{1cm} (2.15)

Species continuity:

\[ \frac{\partial}{\partial x} (\text{r}^A \rho C_i u) + \frac{\partial}{\partial y} (\text{r}^A \rho C_i v) = - \frac{\partial}{\partial y} (\text{r}^A T_j, y) + \text{r}^A w_i \]  \hspace{1cm} (2.16)

\(x\) - Momentum:

\[ \rho \text{r}^A u \frac{\partial u}{\partial x} + \text{r}^A \rho \frac{\partial v}{\partial y} + \rho \text{r}^A uv = - \text{r}^A \frac{\partial P}{\partial x} \]
\[ + \frac{\partial}{\partial y} (\text{r}^A \mu \frac{\partial u}{\partial y}) - \text{r}^A u \frac{\partial \mu}{\partial y} \]  \hspace{1cm} (2.17)

\(y\) - Momentum: \((0[\tilde{\rho}] \text{ and larger terms})\)

\[ \rho \text{r}^A u \frac{\partial v}{\partial x} + \rho \text{r}^A \frac{\partial v}{\partial y} - \rho \text{r}^A u^2 = - \text{r}^A \frac{\partial P}{\partial y} \]
\[ + \frac{\partial}{\partial x} (\text{r}^A \mu \frac{\partial u}{\partial y}) - \frac{2}{3} \frac{\partial}{\partial y} (\mu \frac{\partial \text{r}^A}{\partial x}) + \frac{4}{3} \frac{\partial}{\partial y} (\text{r}^A \mu \frac{\partial v}{\partial y}) \]
\[ - \frac{2}{3} \frac{\partial}{\partial y} (\text{r}^A \mu v + \kappa \text{uv} \frac{\partial \text{r}^A}{\partial y}) \]  \hspace{1cm} (2.18)
TABLE 2.3 (Cont.)

y - Momentum: (0 \[\rho^2\] and larger terms)

\[
\rho x u \frac{\partial v}{\partial x} + \rho x \nu \frac{\partial v}{\partial y} - \rho x A u^2 = - \nu x A \frac{\partial P}{\partial y} \\
+ \frac{\partial}{\partial x} (x A \mu \frac{\partial u}{\partial y}) - \frac{2}{3} \frac{\partial}{\partial y} (\mu \frac{\partial x A u}{\partial x}) + \frac{4}{3} \frac{\partial}{\partial y} (\nu x A \mu \frac{\partial v}{\partial y}) \\
- \frac{2}{3} \frac{\partial}{\partial y} (\nu x A \nu u) - \frac{\partial}{\partial x} (x A \mu u) + \frac{2}{3} \mu \frac{\partial}{\partial x} (x A u) \\
+ \frac{2}{3} \mu \frac{\partial}{\partial y} (\nu x A \nu) - 2 \mu \frac{\partial}{\partial x} (x A \mu u) - \frac{2}{3} \frac{\partial}{\partial y} (\nu x \mu u \frac{\partial x A}{\partial y})
\]

Energy:

\[
x A \rho u \frac{\partial H}{\partial x} + \nu x A \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \left[ \nu x A \left\{ -k \frac{\partial T}{\partial y} + \sum h_i J_{i,y} \right\} \right] - \nu x A \frac{\partial q_{R,y}}{\partial y} \\
- \frac{\rho^2}{N^2} \sum_{i,j \neq i} \frac{N_i}{m_i} \frac{\partial}{\partial P_{ij}} \left( \frac{J_{i,y}}{\rho_j} - \frac{J_{i,y}}{\rho_i} \right) - \nu x A \mu u \frac{\partial u}{\partial y} - \frac{\partial}{\partial y} (\nu x A \mu u)^2
\]
TABLE 2.4  
FIRST ORDER SHOCK LAYER EQUATIONS  

(Order determined at $R_e = \rho_\infty U_\infty R / \mu_{\delta,0} = 100$)

Global continuity:

$$\frac{\partial}{\partial x} (\rho x A u) + \frac{\partial}{\partial y} (\rho x A v) = 0$$  \hspace{1cm} (2.21)

Species continuity:

$$\frac{\partial}{\partial x} (\rho x A_i u) + \frac{\partial}{\partial y} (\rho x A_i v) = - \frac{\partial}{\partial y} (\nu x A_j i, y) + \nu x \omega_i$$  \hspace{1cm} (2.22)

x - Momentum:

$$\rho x A_i \frac{\partial u}{\partial x} + \rho x A_i \frac{\partial v}{\partial y} = - \frac{\partial}{\partial x} (\nu x A j i, y) + \nu x \omega_i$$  \hspace{1cm} (2.23)

y - Momentum:

$$\rho x u^2 = \nu \frac{\partial P}{\partial y}$$  \hspace{1cm} (2.24)

Energy:

$$\rho x A_i \frac{\partial H}{\partial x} + \nu x \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \left( \frac{\rho x A_i}{\nu x A_j i, y} \right) - \frac{\partial}{\partial y} \left( \nu x A \left\{ \sum_i h_j i, y \right\} \right)$$

$$- \frac{P}{2} \sum_i \Sigma \frac{N_i}{m_i} \frac{D_i}{D_i} \left( \frac{J_{i,i} j_i - \frac{J_{i,j} j_j}}{\rho_i} \right) \right) \right) \right) - \nu x A \frac{\partial R_i j_i y}{\partial y}$$  \hspace{1cm} (2.25)

$$+ \frac{\partial}{\partial y} \left( \nu x A_i \frac{\partial u}{\partial y} \right)$$
are of the order of $10^4$ making second order terms even less significant than was shown by the order of magnitude analysis; (2) there are inherent approximations in the theoretical models and experimental data used to predict thermodynamic, transport, radiation and chemical kinetics properties; therefore, there is no need for more detail in the equations solved than in the properties used in the equations.

Further simplification of the conservation equations was obtained by noticing that for the flight conditions and body radii of interest in this work the shock layer is very thin, therefore the relation $K = 1 + \kappa y$ may be approximated by $\kappa = 1$. In addition, neglecting thermal diffusion yields the so-called boundary layer equations (Table 2.5).

**BOUNDARY CONDITIONS**

As was mentioned above, the boundary layer equations are parabolic and thus require the specification of boundary conditions on the stagnation line ($x = 0$), wall ($y = 0$) and shock ($y = \delta$). The stagnation line boundary conditions are obtained by taking the limit of Eqs. 2.26 - 2.30 as $x \to 0$. The resulting equations form the basis for most of the work performed in this dissertation and they will be developed in the next section. Wall and shock boundary conditions will be discussed below.

**Wall Boundary Conditions**

The development of wall boundary conditions may be performed in two different ways. The first, and most frequently used technique

---

*For typical entry conditions of $U_\infty^* = 50,000$ fps, $\rho_\infty^* = 10^{-5}$ 1bm/ft$^3$ (corresponding to an altitude of 214,000 ft (Ref. 2.4)) and $R^* = 10^5$, a value of $T_\delta^* = 15,000$ K is obtained, therefore $\mu_\delta^* = 10^{-4}$ 1bm/ft sec (Ref. 2.5) and $Re = \frac{\rho_\infty^* R^* \ U_\infty^*}{\mu_\delta^*} = 5 \times 10^4$.**
TABLE 2.5
BOUNDARY LAYER EQUATIONS

Global continuity:

\[ \frac{\partial}{\partial x} (r_w A \rho u) + r_w A \frac{\partial}{\partial y} (\rho v) = 0 \]  \hspace{1cm} (2.26)

Species continuity:

\[ \frac{1}{r_w} \frac{\partial}{\partial x} (r_w A \rho C_i u) + \frac{\partial}{\partial y} (\rho C_i v) = - \frac{\partial}{\partial y} (J_{i,x,y}) + \omega_i \]  \hspace{1cm} (2.27)

x - Momentum:

\[ \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = - \frac{\partial P}{\partial x} + \frac{\partial}{\partial y} (\mu \frac{\partial u}{\partial y}) \]  \hspace{1cm} (2.28)

y - Momentum:

\[ 0 = \frac{\partial P}{\partial y} \]  \hspace{1cm} (2.29)

Energy:

\[ \rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} (k \frac{\partial T}{\partial y}) - \frac{\partial}{\partial y} \left\{ \sum_i h_i J_{i,x,y} \right\} - \frac{\partial q_{R,i,y}}{\partial y} \]  \hspace{1cm} (2.30)

\[ + \frac{\partial}{\partial y} (\mu \frac{\partial u}{\partial y}) \]
consists of writing mass, momentum, and energy balances across the ablator-shock layer interface (Fig. 2.2). A second technique involves the use of the conservation equations of the flow-field which are integrated from \( y^+ \) to \( y^- \) and then the resulting equations are evaluated as \( Ay \to 0 \). Both of these methods should yield identical results since the conservation equations used in the second technique are mass, momentum, and energy balances at any point in the flow-field. The first method has the advantage that the physical significance of each term in the resulting equations is more readily evident. The second technique, on the other hand will assure that all the necessary terms have been considered.

In this work the second technique discussed above was applied to the boundary layer equations (Eqs. 2.26 - 2.30) in order to obtain the surface balances needed. For example, the global continuity equation is multiplied by \( dy \) and integrated from \( y^+ \) to \( y^- \)

\[
\int_{y^-}^{y^+} \frac{1}{r_w} \frac{\partial (r_w \rho u)}{\partial y} \, dy + \int_{y^-}^{y^+} \frac{\partial (\rho v)}{\partial y} \, dy = 0
\]

to yield

\[
\left[ \frac{1}{r_w} \frac{\partial (r_w \rho u)}{\partial x} \right]_{av} \Delta y + (\rho v)^+ - (\rho v)^- = 0
\]

where \( \Delta y = y^+ - y^- \) and use has been made of the mean value theorem to integrate the first term. When the limit as \( \Delta y \to 0 \) of the equation above is taken the result is

\[
(\rho v)^- = (\rho v)^+
\]  

(2.31)

This same procedure was used with the other equations and the resulting relations are given in Table 2.6.
Figure 2.2 Illustration of Overall Surface Material Balance
TABLE 2.6
SURFACE BALANCE EQUATIONS

Global Mass Balance:

\[(\rho v)^- = (\rho v)^+ \quad (2.31)\]

Species Mass Balance:

\[(\rho v c_i - J_i)^- = (\rho v c_i - J_i)^+ \quad (2.32)\]

X-momentum:

\[(\rho u - \mu \frac{\partial u}{\partial y})^- = (\rho u - \mu \frac{\partial u}{\partial y})^+ \quad (2.33)\]

y-momentum:

\[p^- = p^+ \quad (2.34)\]

Energy:

\[(\rho v H - k \frac{\partial T}{\partial y} + \sum h_i J_i, y + q_{R,y} - \mu u \frac{\partial u}{\partial y})^- \quad (2.35)\]

\[= (\rho v H - k \frac{\partial T}{\partial y} + \sum h_i J_i, y + q_{R,y} - \mu u \frac{\partial u}{\partial y})^+\]
In these surface balance equations all the dependent variables on
the char side of the interface (those with a superscript -) must be in-
terpreted as being dependent upon both the solid and gaseous phases. For
example \( \rho^{-} = \rho_g + \rho_c \) and \( (\rho v)^{-} = \rho_g v_g + \rho_c v_c \). In addition it must be no-
ticed that if the flow in the char is one dimensional \( (u^{-} = 0) \), as it is
usually assumed to be, the \( x \) - momentum equation is identically zero
while the terms with arrows through them in the energy balance also be-
come zero. This same situation exists on the stagnation line since \( u \)
is zero for all values of \( y \).

Shock Boundary Conditions

The bow shock is governed by three basic conservation equations,
corresponding to the three physical principles of conservation of mass,
momentum, and energy. These equations, commonly known as the Rankine-
Hugoniot equations are given in rectangular coordinates by (Ref. 2.6):

**Continuity**

\[
\rho_{\infty} \frac{V_{\infty}}{\delta_n} = \rho_0 \frac{V_0}{\delta_n} \tag{2.36}
\]

**Momentum**

(normal) \( \rho_{\infty} + \rho_0 \frac{V_{\infty}^2}{\delta_n} = \rho_0 \frac{V_0^2}{\delta_n} \tag{2.37} \)

(tangential) \( V_{\infty} t = V_0 t \tag{2.38} \)

**Energy**

\[
h_{\infty} + \frac{1}{2} V_{\infty}^2 + \frac{1}{2} \frac{V_0^2}{\delta_n} = h_0 + \frac{1}{2} \frac{V_0^2}{\delta_n} + \frac{1}{2} \frac{V_0^2}{\delta_n} \tag{2.39}
\]

Using Figure 2.3 the above equations can be written in body oriented co-
ordinates. The development of these equations in curvilinear coordinates
was performed by Engel (Ref. 2.1) and the resulting equations are given
below in dimensionless form

\[
v_0 = \sin \phi \sin \epsilon - \rho \cos \phi \cos \epsilon \tag{2.40}
\]

\[
u_0 = \sin \phi \cos \epsilon - \rho \cos \phi \sin \epsilon \tag{2.41}
\]
Figure 2.3 Resolution of Velocity Components in a Body-Oriented Coordinate System
\[ P_\delta = (1-\rho) \cos^2 \phi + P_\infty^0 \]  
\[ h_\delta = (1-\rho^2) \cos \phi + h_\infty^0 \]  
\( (2.42) \)  
\( (2.43) \)

Again, the dimensionless variables used above were defined as given in Table 2.2. As shown in Eqs. 2.42 and 2.43 the terms \( P_\infty \) and \( h_\infty \) may be neglected since they are of order \( \rho^{-2} \).

For a given shock shape and flight conditions, if the post-shock fluid is assumed to be pure air in chemical equilibrium, i.e., no diffusion of ablation products to the shock, then the velocity of the fluid at the shock and also its thermodynamic state (pressure, enthalpy, composition, etc.) can be found from Eqs. 2.40 - 2.43 and a technique for obtaining the equilibrium composition of a fluid. In practice a chemical equilibrium program is usually available and a value of \( \tilde{\rho} \) is guessed, from Eqs. 2.42 and 2.43 \( P_\delta \) and \( h_\delta \) are computed and the equilibrium program is used to obtain the composition and a new value of \( \tilde{\rho} \) is obtained. This procedure is repeated until the guessed and computed values of \( \tilde{\rho} \) agree.

Therefore, boundary conditions of the first kind, i.e., the dependent variables are specified, may be used at the shock \( (y = \delta) \). These boundary conditions are given below

\[ u = u_\delta \]  
\[ v = v_\delta \]  
\[ P = P_\delta \]  
\[ h = h_\delta \]  
\[ C_i = C_i^\delta (P , h) \]  
( Assuming chemical equilibrium )  
\[ I_{\tilde{y}}(T_w^\delta) = 0 \]  
( No precursor radiation )

The additional boundary condition shown above results from assuming that no radiation from the free-stream air crosses the shock.
STAGNATION LINE BOUNDARY LAYER EQUATIONS*

The stagnation line boundary layer equations are obtained by formally taking the limit as \( x \to 0 \) of the boundary layer equations (Eqs. 2.26 - 2.30). The resulting equations were obtained by Engel (Ref. 2.1) and are given here in dimensional form for axisymmetric flow in Table 2.7. Some comments concerning the derivation of the equations in Table 2.7 are pertinent: 1) at the stagnation line the component of velocity tangential to the body (\( u \)) is zero because of symmetry; 2) the stagnation line \( x \)-momentum equation is obtained by first differentiating the \( x \)-momentum equation (Eq. 2.28) with respect to \( x \) and then taking the limit as \( x \to 0 \) of the resulting equation. This procedure is used because taking the limit of the \( x \)-momentum equation yields \( (\partial P/\partial x)_x = 0 \), a relationship which does not contain any useful information.

The wall and shock boundary conditions needed in order to be able to integrate Eqs. 2.45 - 2.49 were obtained by taking the limit of Eqs. 2.31 - 2.35 and 2.40 - 2.43 as \( x \to 0 \). Before taking the limit of the surface balance equations the flow in the char was assumed to be one-dimensional (\( u^+ = u^- = 0 \)). As was discussed earlier, this condition implies that the terms crossed by an arrow in the energy balance equation are zero while the \( x \)-momentum balance is identically zero. In lieu of the \( x \)-momentum balance, the fact that \( u \) is zero for all \( x \) locations at the wall ((\( \partial u/\partial x \)) = 0) may be used with the stagnation line global continuity equation (Eq. 2.45) to yield

\[
\frac{\partial (\rho u')^+}{\partial y} = 0
\]

*In this section all variables are dimensional.
**TABLE 2.7**  
**STAGNATION LINE BOUNDARY LAYER EQUATIONS**

Global continuity:

\[
2 \frac{\partial u}{\partial x} = - \frac{1}{\rho} \frac{\partial}{\partial y} (\rho v) \tag{2.45}
\]

Species continuity:

\[
\rho v \frac{\partial C_i}{\partial y} = - \frac{\partial}{\partial y} (J_{i,y}) + w_i \tag{2.46}
\]

**x - Momentum:**

\[
\frac{\partial}{\partial y} \left[ \mu \frac{\partial}{\partial y} \left( \frac{1}{\rho} \frac{\partial}{\partial y} (\rho v) \right) \right] - \rho v \frac{\partial}{\partial y} \left( \frac{1}{\rho} \frac{\partial}{\partial y} (\rho v) \right) + \frac{\partial}{\partial y} \left( \frac{1}{\rho} \frac{\partial}{\partial y} (\rho v) \right)^2 + 2 \left( \frac{\partial^2 P}{\partial x^2} \right)_{x=0} = 0 \tag{2.47}
\]

**y - Momentum:**

\[
\frac{\partial P}{\partial y} = 0 \tag{2.48}
\]

**Energy:**

\[
\rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \left[ - k \frac{\partial T}{\partial y} + \sum_i h_i J_{i,y} \right] - \frac{\partial q_{R,v}}{\partial y} \tag{2.49}
\]
The stagnation line wall boundary conditions are given in Table 2.8. At the shock \( \phi = 0 \) and the shock boundary conditions simplify to those given in Table 2.8. The reader should notice that while all the shock boundary conditions are of the first kind, the wall boundary conditions are of the first, second and third kind.

**MATHEMATICAL DESCRIPTION OF THE PROBLEM**

Before any attempt is made to describe the mathematics of the problem, it is convenient to introduce into the equations the binary diffusion assumption

\[
J_{i,y} = -\rho D \frac{\partial C_i}{\partial y} \quad (i = 1, \ldots, n) \tag{2.51}
\]

and use the relation

\[
H = h + \frac{v^2}{2} \tag{2.52}
\]

to write the energy equation (Eq. 2.49) in terms of static enthalpy instead of total enthalpy. When this is done the resulting conservation equations are:

- **Global continuity:**
  \[
  2 \left( \frac{\partial u}{\partial x} \right)_{x=0} = -\frac{1}{\rho} \frac{d(\rho v)}{dy} \tag{2.45}
  \]

- **Species continuity:**
  \[
  \frac{dC_i}{dy} + \rho v \frac{dC_i}{dy} + \omega_i = 0 \quad (i = 1, \ldots, n) \tag{2.53}
  \]

- **x - momentum:**
  \[
  \frac{1}{\rho} \frac{d(\rho v)}{dy} - \rho v \frac{d(\rho v)}{dy} \frac{1}{\rho} \frac{d(\rho v)}{dy} \left( \frac{1}{\rho} \frac{d(\rho v)}{dy} \right) \tag{2.47}
  \]

  \[
  + \frac{\rho}{2} \frac{1}{\rho} \frac{d(\rho v)}{dy} + \frac{\partial^2 p}{\partial x^2} \mid_{x=0} = 0
  \]
TABLE 2.8

WALL AND SHOCK BOUNDARY CONDITIONS FOR STAGNATION LINE PROBLEM

Wall \( (y = 0) \): 
\[
\rho v = (\rho v)^- \hspace{1cm} (2.50a)
\]
\[
\rho v c_i - J_i = (\rho v c_i - J_i)^- \hspace{1cm} (2.50b)
\]
\[
\frac{\partial (\rho v)}{\partial y} = 0 \hspace{1cm} (2.50c)
\]
\[
P = P^- \hspace{1cm} (2.50d)
\]
\[
(\rho v H - k \frac{\partial T}{\partial y} + \Sigma h_i J_i, y + q_{R,y}) = \hspace{1cm} (2.50e)
\]
\[
(\rho v H - k \frac{\partial T}{\partial y} + \Sigma h_i J_i, y + q_{R,y})^- \hspace{1cm} (2.50e)
\]

Shock \( (y = \delta) \): 
\[
v = v_\delta = - \frac{\rho_\infty}{\delta,0} U_\infty \cos \epsilon \hspace{1cm} (2.50f)
\]
\[
u = u_\delta \frac{P_\infty U_\delta,0}{P_{\delta,0}} \sin \epsilon \hspace{1cm} (2.50g)
\]
\[
P = P_\delta = (1 - \frac{\rho_\infty}{\rho_{\delta,0}}) \rho_\infty U_\infty \hspace{1cm} (2.50h)
\]
\[
h = h_\delta = (1 - (\frac{\rho_\infty}{\rho_{\delta,0}})^2 \frac{U_\infty}{2} \hspace{1cm} (2.50i)
\]
\[
C_1 = C_i (p_{\delta,0}, h_\delta) \hspace{1cm} (2.50i)
\]
y - momentum:

\[
\frac{dP}{dy} = 0 \quad (2.48)
\]

Energy:

\[
\rho v \frac{dh}{dy} + \rho v^2 \frac{dv}{dy} = \frac{d(k \frac{dT}{dy})}{dy} - \left( \rho \frac{\partial}{\partial y} \frac{n}{i} \frac{dC_i}{dy} \right)
\]

\[
- \frac{dq_{r,y}}{dy} \quad (2.54)
\]

The mathematical model of the stagnation line is given by the above set of 4 + n (for a system with n chemical species) ordinary integro-differential equations and a set of two-point boundary conditions given in Table 2.8. The integro-differential equations are coupled, nonlinear, of first, second and third order. They are integral since the flux divergence term (\( dq_{r,y} /dy \)) in the energy equation is an integral given by Eq. 2.14. These equations contain the 7 + n unknowns \( \rho, v, (\partial u/\partial x)_{x=0}, P, h, T, \) and \( C_i \) (\( i = 1, \ldots, n \)) where both \( (\partial u/\partial x)_{x=0} \) and \( (\partial^2 P/\partial x^2)_{x=0} \) are at most functions of y. This discussion assumes that thermodynamic, transport, radiative, and kinetics properties \( (D, \omega, \mu, k, \) and \( h_i) \) are known in terms of the dependent variables listed above. These properties will be discussed in Chapter 3. It is evident that since the 4 + n equations contain 7 + n unknowns three more independent relations are needed. These are provided by the thermal equation of state

\[
P = \left( \frac{\rho C_i}{M_i} \right) \rho RT \quad (2.55)
\]

the caloric equation of state;

\[
h = \left( \frac{\rho}{M_i} \right) C_i h_i \quad (2.56)
\]
and the Rankine-Hugoniot relation for the shock pressure as a function of the shock angle measured from the stagnation line

\[ p_\delta = (1 - \bar{\rho}) \cos^2 \phi_\alpha \ U_\infty^2 \]  
(2.42)

From the y-momentum equation and the fact that \( \frac{\partial F}{\partial x} \bigg|_{x = 0} \) (as discussed in the previous section) it is evident that

\[ \frac{\partial^2 p}{\partial x^2} \bigg|_{x = 0} = \frac{\partial^2 p_\delta}{\partial x^2} \bigg|_{x = 0} = \text{constant} \]  
(2.57)

Substitution of Eq. 2.42 in Eq. 2.57 gives

\[ \frac{\partial^2 p}{\partial x^2} \bigg|_{x = 0} = -2 (1 - \bar{\rho}) \left( \frac{\partial \phi}{\partial x} \right)^2 = 0 \]  
(2.58)

This development makes it possible to rewrite the x-momentum equation as

\[ \frac{\partial^2 \rho v}{\partial x^2} = \rho v \frac{\partial^2 \rho v}{\partial y^2} - \rho v \frac{1}{\rho} \frac{d \rho v}{dy} - \frac{1}{\rho} \frac{d \rho v}{dy} \]  
(2.59)

\[ + \frac{\theta}{2} \left( \frac{d \rho v}{dy} \right)^2 - 4 (1 - \bar{\rho}) \left( \frac{\partial \phi}{\partial x} \right)^2 = 0 \]  

Therefore, for a known shock geometry (known \( \phi(x) \)) the conservation equations contain \( 6 + n \) unknowns instead of \( 7 + n \) as before. A further reduction in the number of equations that need to be solved may be accomplished by eliminating \( h \) from the energy equation by substituting the caloric equation of state as follows. From Eq. 2.56

\[ \frac{dh}{dy} = \sum_i h_i \frac{dC_i}{dy} + \sum_i C_i \frac{dh_i}{dy} \]  
(2.60)

\[ = \sum_i h_i \frac{dC_i}{dy} + (\sum_i C_i \frac{dh_i}{dT}) \frac{dT}{dy} \]
Substituting Eq. 2.60 in Eq. 2.54 gives

\[ n \sum_i h_i \frac{dC_i}{dy} + \left( \sum_i C_i \frac{C_p}{C} \right) \frac{dT}{dy} \]

\[ = n \sum_i h_i \frac{dC_i}{dy} + C_p \frac{dT}{dy} \]

Energy:

\[ \rho v \frac{d^2 \rho}{dy} = - \rho v^2 \frac{dv}{dy} - \rho v \left( \sum_i h_i \frac{dC_i}{dy} \right) \]

\[ + \frac{d[2k \frac{dT}{dy} + \rho \left( \sum_i h_i \frac{dC_i}{dy} \right) \cdot dq_{R,y}]}{dy} - \frac{dq_{R,y}}{dy} \] \hspace{1cm} (2.61)

In this manner the unknowns have been reduced to \( \rho, v, (\partial u/\partial x)_x = 0, \)

\( \mathcal{P}, T, \) and \( C_i \) (\( i = 1, \ldots, n \)).

At this point it is pertinent to ask, how many of Eqs. 2.45, 2.53, 2.48, 2.55, 2.59, and 2.61 must be solved simultaneously? It is evident that the \( y \)-momentum equation (Eq. 2.48), containing only one dependent variable, is not coupled to the other equations. In fact, it can be integrated analytically to yield

\[ P(y) = P_0 = \text{constant} \] \hspace{1cm} (2.62)

In addition, the global continuity equation (Eq. 2.45) contains only two dependent variables and can be left out of the set that must be solved initially. This has the effect of eliminating \( (\partial u/\partial x)_x = 0 \) from the unknowns in the equations that must be solved. This variable may be readily obtained from Eq. 2.45 once the \( \rho \) and \( v \) profiles are known. The answer to the question that was asked at the beginning of this paragraph is that Eqs. 2.53, 2.55, and 2.59, and 2.61 in the unknowns \( \rho, v, T, \) and \( C_i \) (\( i = 1, \ldots, n \)) must be solved simultaneously.
Let us now consider the boundary conditions that must be used with these equations. The species continuity equation (Eq. 2.53) being second order requires two boundary conditions for \( C_i \). These may be provided by Eqs. 2.50 b and 2.50 j

\[
\rho v C_i + \frac{dC_i}{dy} = (\rho v C_i + \rho D \frac{dC_i}{dy})^- \text{ at } y = 0 \tag{2.63}
\]

\[
C_i = C_i, \delta \text{ at } y = \delta \tag{2.50j}
\]

Notice that the binary diffusion assumption (Eq. 2.51) was substituted in Eq. 2.50b to obtain Eq. 2.63. The x-momentum equation (Eq. 2.59) is third order and requires three boundary conditions for \( \rho v \). These are given by Eqs. 2.50a, 2.50c,

\[
\rho v = (\rho v) w \text{ at } y = 0 \tag{2.50a}
\]

\[
\frac{d(\rho v)}{dy} = 0 \text{ at } y = 0 \tag{2.50c}
\]

and

\[
\rho v = \rho_{\delta} v_{\delta} \text{ at } y = \delta \tag{2.64}
\]

The energy equation (Eq. 2.61) being second order in \( T \) requires two boundary conditions in addition to the ones already discussed in connection with radiation. The first of these boundary conditions is provided by the wall energy balance (Eq. 2.50e), this relation is written in terms of the variables previously discussed by substituting Eqs. 2.51, 2.52 and 2.56

\[
\rho v (n \Sigma C_i h_i + \frac{v^2}{2}) - k \frac{dT}{dy} - \rho D (n \Sigma \frac{h_i dC_i}{dy}) + q_{R,y} = \]

\[
[\rho v (n \Sigma C_i h_i + \frac{v^2}{2}) - k \frac{dT}{dy} - \rho D (n \Sigma \frac{h_i dC_i}{dy}) + q_{R,y}]^- \tag{2.65}
\]
The second temperature boundary condition needed is given by

\[ T = T_\delta \text{ at } y = \delta \]  

(2.65)

This completes the boundary conditions needed. Of these the most complex ones are those given by Eqs. 2.63 and 2.65. The boundary condition given by Eq. 2.63 may be simplified by noticing that for fairly high mass injection rates \((\rho v)_\text{wall}/\rho_u U > 0.05\) mass transfer by diffusion is small compared to mass transfer by convection near the wall.

This means that the diffusion terms in Eq. 2.63 may be neglected to yield

\[ C_i = C_i^- \text{ at } y = 0 \quad (i = 1, \ldots, n) \]  

(2.67)

where use has been made of Eq. 2.50a to cancel the \(\rho v\) terms from the equation above. The wall energy balance (Eq. 2.65) may also be simplified by neglecting the kinetic energy of the fluid \(v^2/2\) since it is small when compared to the thermal energy. When this is done Eq. 2.65 becomes

\[ \rho v \left( \sum_i^n C_i h_i \right) - k \frac{dT}{dy} - \rho D \left( \sum_i^n h_i \frac{dC_i}{dy} \right) + q = \]  

(2.68)

\[ \left[ \rho v \left( \sum_i^n C_i h_i \right) - k \frac{dT}{dy} - \rho D \left( \sum_i^n h_i \frac{dC_i}{dy} \right) + q \right]^- \]

Since all the other boundary conditions are of the are of the first and second kind and uncoupled, while Eq. 2.68 is of the third kind and coupled to the species continuity equation, it was expedient to assume that the char is at the sublimation temperature of carbon:

\[ T = T_w \text{ at } y = 0 \]  

(2.69)

Until now we have assumed that \(\delta\) (the shock stand-off distance) is known, a necessary condition to be able to integrate the equations of the flow-field. In practice, \(\delta\) is unknown and therefore must be guessed to be able to compute it correctly. This boundary condition is obtained by
evaluating the global continuity equation at the shock

\[ \frac{d(pu)}{dy} = -2 \int_{x_0}^{x_{\delta}} \left( \frac{\partial u}{\partial x} \right)_{x=0} \ \text{at} \ y = \delta \quad (2.70) \]

Table 2.9 gives a summary of the stagnation line model including the conservation equations, the equation of state and the boundary conditions.

REFERENCES

2.1 Engel, Carl D., Ablation and Radiation Coupled Viscous Hypersonic Shock Layers, Ph.D. Dissertation, Louisiana State University, Baton Rouge, Louisiana (1971)


TABLE 2.9

SUMMARY OF THE STAGNATION LINE MODEL

Governing Equations:

Species continuity:

\[
\frac{dC_i}{dy} - \rho v \frac{dC_i}{dy} + \omega_i = 0
\]  

(2.53)

X-momentum:

\[
\frac{d}{dy} \left[ \frac{1}{\rho} \frac{d(\rho v)}{dy} \right] - \rho v \frac{d(\rho v)}{dy} + \frac{1}{\rho} \frac{d(\rho v)}{dy}^2 - 4 (1-\bar{\rho}) \left( \frac{\partial v}{\partial x} \right)_x = 0
\]

(2.59)

Energy:

\[
\frac{d(k)}{dy} - \rho v c_p \frac{dT}{dy} + \frac{d(\rho v)}{dy} \left[ \sum_i \frac{n_i}{M_i} \frac{dC_i}{dy} \right] - \rho v \frac{2}{dy} \frac{dv}{dy} - \rho v \left( \sum_i h_i \frac{dC_i}{dy} \right) - \frac{dQ_y}{dy} = 0
\]

(2.61)

Thermal equation of state:

\[
\rho \frac{n}{\bar{M}} \frac{C_i}{d} = \rho \frac{n}{\bar{M}} \frac{C_i}{d} = \frac{\delta}{\delta}
\]

(2.55)
Boundary Conditions:

Wall \((y = 0)\)  

1. \(\rho \nu = (\rho \nu)_w\) \hspace{1cm} (2.50a) 

2. \(\frac{d(\rho \nu)}{dy} = 0\) \hspace{1cm} (2.50c) 

3. \(C_\perp = C_{\perp w}\) \hspace{1cm} (2.67) 

4. \(T = T_w\) \hspace{1cm} (2.68) 

Shock \((y = \delta)\)  

1. \(\rho \nu = (\rho \nu)_{\delta}\) \hspace{1cm} (2.64) 

2. \(\frac{d(\rho \nu)}{dy} = -2\rho_{\delta,0} \left( \frac{\partial u_{\delta}}{\partial x} \right)_{x=0}\) \hspace{1cm} (2.70) 

3. \(C_\perp = C_{\perp \delta}\) \hspace{1cm} (2.50j) 

4. \(T = T_{\delta}\) \hspace{1cm} (2.69)
CHAPTER 3

THERMODYNAMIC, TRANSPORT, KINETIC,
AND RADIATIVE PROPERTIES

The thermodynamic, transport, kinetic, and radiative properties of the mixture of air and ablation species which are necessary to solve the conservation equations that were presented in the previous chapter are evaluated with the methods described in this chapter.

THERMODYNAMIC PROPERTIES

Thermodynamic Properties of Pure Species at Standard State

The specific heat at constant pressure, enthalpy, entropy, and Gibbs free energy of the pure species at one atmosphere pressure (standard state) were obtained by Esch, et. al. (Ref. 3.1). This was accomplished by curve fitting with the method of least squares, temperature polynomials to data found in the literature. The polynomials used to fit the thermodynamic properties are given in Table 3.1. For each species, two different fits were made, one for low temperatures \((1000^\circ K < T < 6000^\circ K)\) and the other for high temperatures \((6000^\circ K < T < 15,000^\circ K)\). For each species, the coefficients for the expressions in Table 3.1 are given in Table 3.2 for the two temperature ranges. Each term in Eqs. 3.1 - 3.4 is dimensionless, temperature is in \(^{\circ}K\) and \(R = 1.987 \text{ cal/gmole} - ^{\circ}K\), therefore the units of the thermodynamic properties are as given below

\[ C_{pi} = [\text{cal/gmole of } i - ^{\circ}K] \]
TABLE 3.1 POLYNOMINAL EQUATIONS FOR STANDARD THERMODYNAMIC PROPERTIES

**Specific Heat**

\[ C_{p,i}^0 \frac{1}{R} = A_{1,i} + A_{2,i}T + A_{3,i}T^2 + A_{4,i}T^3 + A_{5,i}T^4 \]  \hspace{1cm} (3.1)

**Enthalpy**

\[ h_{i}^0 \frac{1}{RT} = A_{1,i} + \frac{A_{2,i}T}{2} + \frac{A_{3,i}T^2}{3} + \frac{A_{4,i}T^3}{4} + \frac{A_{5,i}T^4}{5} + \frac{A_{6,i}}{T} \]  \hspace{1cm} (3.2)

**Entropy**

\[ S_{i}^0 \frac{1}{R} = A_{1,i}lnT + A_{2,i}T + \frac{A_{3,i}T^2}{2} + \frac{A_{4,i}T^3}{3} + \frac{A_{5,i}T^4}{4} + A_{7,i} \]  \hspace{1cm} (3.3)

**Free Energy**

\[ F_{i}^0 \frac{1}{RT} = A_{1,i}(1-lnT) - \frac{A_{2,i}T}{2} - \frac{A_{3,i}T^2}{6} - \frac{A_{4,i}T^3}{12} - \frac{A_{5,i}T^4}{20} + \frac{A_{6,i}}{T} - A_{7,i} \]  \hspace{1cm} (3.4)
## TABLE 3.2

**POLYNOMIAL COEFFICIENTS FOR THERMODYNAMIC PROPERTY CORRELATIONS**

<table>
<thead>
<tr>
<th>Species</th>
<th>A1,_i</th>
<th>A2,_i</th>
<th>A3,_i</th>
<th>A4,_i</th>
<th>A5,_i</th>
<th>A6,_i</th>
<th>A7,_i</th>
<th>T*</th>
</tr>
</thead>
<tbody>
<tr>
<td>C+</td>
<td>0.2609E 01</td>
<td>-0.1393E-03</td>
<td>0.5959E-07</td>
<td>-0.1037E-10</td>
<td>0.6345E-15</td>
<td>0.2168E 06</td>
<td>0.3709E 01</td>
<td>L.</td>
</tr>
<tr>
<td>H</td>
<td>0.2528E 01</td>
<td>0.4869E-05</td>
<td>-0.7026E-08</td>
<td>0.1134E-11</td>
<td>-0.3476E-16</td>
<td>0.2168E 06</td>
<td>0.4139E 01</td>
<td>H.</td>
</tr>
<tr>
<td>N+</td>
<td>0.2727E 01</td>
<td>-0.2620E-03</td>
<td>0.1105E-06</td>
<td>-0.1561E-10</td>
<td>0.7847E-15</td>
<td>0.2254E 06</td>
<td>0.3645E 01</td>
<td>L.</td>
</tr>
<tr>
<td>O+</td>
<td>0.2944E 01</td>
<td>-0.4108E-03</td>
<td>0.9156E-07</td>
<td>-0.1190E-15</td>
<td>0.1879E 06</td>
<td>0.4424E 01</td>
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<tr>
<td>E-</td>
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<td>0.3440E-06</td>
<td>-0.1954E-09</td>
<td>0.3937E-13</td>
<td>-0.2573E-17</td>
<td>-0.7450E 03</td>
<td>-0.1173E 02</td>
<td>L.</td>
</tr>
<tr>
<td>C</td>
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<td>-0.6332E-05</td>
<td>0.1364E-08</td>
<td>-0.1094E-12</td>
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<td>-0.7450E 03</td>
<td>-0.1208E 02</td>
<td>H.</td>
</tr>
<tr>
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<td>0.1095E-06</td>
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<td>L.</td>
</tr>
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<td>CN</td>
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<td>-0.5498E-07</td>
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<td>-0.5564E-16</td>
<td>0.8542E 05</td>
<td>0.5874E C1</td>
<td>H.</td>
</tr>
<tr>
<td>CO</td>
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<td>0.4897E-03</td>
<td>-0.1055E-06</td>
<td>-0.3475E-10</td>
<td>0.2361E-14</td>
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</tr>
<tr>
<td>C2</td>
<td>0.3473E C1</td>
<td>0.7337E-03</td>
<td>-0.9038E-07</td>
<td>0.4847E-11</td>
<td>-0.1018E-15</td>
<td>0.5420E 05</td>
<td>0.4152E C1</td>
<td>H.</td>
</tr>
<tr>
<td>C2H</td>
<td>0.3254E C1</td>
<td>0.9698E-03</td>
<td>-0.2647E-06</td>
<td>0.3037E-10</td>
<td>-0.1177E-14</td>
<td>0.4745E 05</td>
<td>0.5809E 05</td>
<td>0.4784E C1</td>
</tr>
<tr>
<td>C2H</td>
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<td>0.8027E-03</td>
<td>-0.1968E-06</td>
<td>0.1940E-10</td>
<td>-0.1048E-15</td>
<td>0.1434E 05</td>
<td>0.4875E C1</td>
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<tr>
<td>C2H</td>
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<td>0.3036E-06</td>
<td>-0.6244E-10</td>
<td>0.3915E-14</td>
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<td>0.5288E C1</td>
<td>H.</td>
</tr>
<tr>
<td>C2H</td>
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<td>-0.7026E-07</td>
<td>0.4666E-11</td>
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<td>0.1090E C1</td>
<td>H.</td>
</tr>
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<td>C2H</td>
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<td>0.3563E-02</td>
<td>-0.1237E-05</td>
<td>0.1866E-09</td>
<td>-0.1013E-13</td>
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<td>0.4784E C1</td>
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<td>0.5809E 05</td>
<td>0.5288E C1</td>
<td>H.</td>
</tr>
</tbody>
</table>

* Temperature Range L = 1000-6000K, H = 6000-15000K
<table>
<thead>
<tr>
<th>Species</th>
<th>$A_1,i$</th>
<th>$A_2,i$</th>
<th>$A_3,i$</th>
<th>$A_4,i$</th>
<th>$A_5,i$</th>
<th>$A_6,i$</th>
<th>$A_7,i$</th>
<th>$T^*$</th>
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<tbody>
<tr>
<td>C$_2$H$_2$</td>
<td>$0.3891E+01$</td>
<td>$0.5717E-02$</td>
<td>$-0.1957E-05$</td>
<td>$0.2931E-09$</td>
<td>$-0.1585E-13$</td>
<td>$0.2590E+05$</td>
<td>$0.6520E+00$</td>
<td>L</td>
</tr>
<tr>
<td>C$_3$</td>
<td>$0.4002E+01$</td>
<td>$0.3541E-02$</td>
<td>$-0.1318E-05$</td>
<td>$0.2064E-09$</td>
<td>$-0.1144E-13$</td>
<td>$0.9423E+05$</td>
<td>$-0.1021E+03$</td>
<td>H</td>
</tr>
<tr>
<td>C$_3$H</td>
<td>$0.2935E+01$</td>
<td>$0.3541E-02$</td>
<td>$-0.1318E-05$</td>
<td>$0.2064E-09$</td>
<td>$-0.1144E-13$</td>
<td>$0.9423E+05$</td>
<td>$-0.1021E+03$</td>
<td>H</td>
</tr>
<tr>
<td>C$_4$H</td>
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<td>$0.7403E-02$</td>
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<td>$0.4437E-09$</td>
<td>$-0.2637E-13$</td>
<td>$0.7605E+05$</td>
<td>$-0.4010E+01$</td>
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</tr>
<tr>
<td>HCN</td>
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<td>$-0.1258E-05$</td>
<td>$0.2169E-09$</td>
<td>$-0.1430E-13$</td>
<td>$0.1442E+05$</td>
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<tr>
<td>H$_2$</td>
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<td>$0.9372E-07$</td>
<td>$-0.2948E-10$</td>
<td>$0.2141E-14$</td>
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<td>$-0.3548E+01$</td>
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</tr>
<tr>
<td>N</td>
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<td>$0.5565E-02$</td>
<td>$-0.1759E-01$</td>
<td>$0.1536E-05$</td>
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<td>$0.9423E+05$</td>
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<td>H</td>
</tr>
<tr>
<td>O</td>
<td>$0.2670E+01$</td>
<td>$0.1970E-03$</td>
<td>$0.7153E-07$</td>
<td>$0.8901E-11$</td>
<td>$0.4005E-16$</td>
<td>$-0.1018E+04$</td>
<td>$-0.3716E+01$</td>
<td>H</td>
</tr>
<tr>
<td>N$_2$</td>
<td>$0.3221E+01$</td>
<td>$0.5952E-04$</td>
<td>$0.2751E-07$</td>
<td>$-0.2798E-11$</td>
<td>$0.9380E-16$</td>
<td>$0.2915E+05$</td>
<td>$0.5049E+01$</td>
<td>H</td>
</tr>
<tr>
<td>O$_2$</td>
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<td>$0.4254E-03$</td>
<td>$-0.2535E-07$</td>
<td>$0.6050E-12$</td>
<td>$-0.5186E-17$</td>
<td>$-0.1044E+04$</td>
<td>$0.3254E+01$</td>
<td>H</td>
</tr>
</tbody>
</table>

*Temperature Range  
L = 1000-6000°K, H = 6000-15,000°K
\[ h_i^\circ = \text{[cal/gmole of } i] \]
\[ S_i^\circ = \text{[cal/gmole of } i - \text{ } ^\circ \text{K}] \]
\[ F_i^\circ = \text{[cal/gmole of } i] \]

**Thermodynamic Properties of Pure Species at Arbitrary State**

Expressions for the thermodynamic properties of pure species at arbitrary pressures and temperatures are predicted in the following manner. The species are assumed to be ideal gases so that (Ref. 3.2)

\[ h_i = h_i (T) = h_i^\circ \] (3.5)

and since \( C_{pi} = (\partial h_i / \partial T)_P \) then

\[ C_{pi} = C_{pi} (T) = C_{pi}^\circ \] (3.6)

In other words, both the enthalpy and the specific heat at constant pressure are independent of pressure. On the other hand let us examine entropy, from the first law of thermodynamics

\[ dh_i = T_i dS_i + \frac{1}{X_i} dP \] (3.7)

where \( X_i \) is the molar concentration of species \( i \) (moles of \( i \)/volume).

Rewriting Eq. 3.7 gives

\[ dS_i = \frac{1}{T_i} dh_i - \frac{1}{X_i T_i} dP \] (3.8)

From the thermal equation of state for an ideal gas

\[ P_i = X_i \frac{RT}{T} \] (3.9)

and Eq. 3.8 can be rewritten as

\[ dS_i = \frac{1}{T_i} dh_i - R d (\ln P) \] (3.10)
and integrated to yield

\[ S_i (T,P) = \frac{1}{T} \int dhi - R \ln P + A_{\delta, i} \]  

(3.11)

where \( A_{\delta, i} \) is an integration constant. In order to evaluate \( A_{\delta, i} \) we make use of the fact that \( S_i (T,1) = S_i^\circ \) and obtain (by evaluating Eq. 3.11 at \( P = 1 \) atmosphere).

\[ A_{\delta, i} = S_i^\circ - \int dhi \]  

(3.12)

Substitution of Eq. 3.12 in Eq. 3.11 yields

\[ S_i = S_i (T,P) = S_i^\circ - R \ln P \]  

(3.13)

The Gibbs free energy is defined as

\[ F_i = h_i - TS_i \]  

(3.14)

substitution of Eqs. 3.5 and 3.13 in the above equation results in

\[ F_i = h_i^\circ - TS_i^\circ - RT \ln P \]  

(3.15)

or

\[ F_i = F_i (T,P) = F_i^\circ + RT \ln P \]  

(3.16)

since

\[ F_i^\circ = h_i^\circ - TS_i^\circ \]

Thermodynamic Properties of Mixtures

For each species in a mixture consisting of a total of \( n \) gaseous species the thermodynamic properties are given by

\[ h_i = h_i (T) = h_i^\circ \]  

(3.17)

\[ C_{pi} = C_{pi} (T) = C_{pi}^\circ \]  

(3.18)

\[ S_i = S_i (T,P) = S_i^\circ - R \ln P_i \]  

(3.19)

\[ F_i = F_i (T,P) = F_i^\circ + RT \ln P_i \]  

(3.20)
where $P_i$ is the partial pressure of species $i$ (atmosphere). Mixture properties are then given by

$$h = \sum_{i} y_i h_i \text{[cal./gmole of mixture]}$$

(3.21)

$$C_p = \sum_{i} y_i C_i \text{[cal./gmole of mixture - °K]}$$

(3.22)

$$S = \sum_{i} y_i S_i \text{[cal./gmole of mixture - °K]}$$

(3.23)

$$F = \sum_{i} y_i F_i \text{[cal./gmole of mixture]}$$

(3.24)

where $y_i$ is the $i$th species mole fraction (gmole of $i$/gmole of mixture) and the units of each property are given by the terms in brackets.

**TRANSPORT PROPERTIES**

Presently available transport properties data for air and ablation products are extremely limited because of the difficulties involved with experimental measurements at the extremely high temperatures of interest. Thus, it is necessary to rely heavily on properties obtained from theoretical predictions like the Chapman-Enskog kinetic theory (Ref. 3.3). At the lower temperatures, where ionization has not yet begun to occur, the classical first order Chapman-Enskog kinetic theory has been found to be reasonably accurate. However for higher temperatures the use of more rigorous kinetic models becomes necessary. The transport properties used in the present work were obtained by Esch (Ref. 3.4); in order to obtain simple closed form expressions for species viscosity and thermal conductivity the theoretical results reported in the literature were curve fit with polynomial expressions in temperature.

**Viscosity**

The species viscosity data obtained from theoretical predictions
were curve fit to a second degree polynomial in temperature

\[ \mu_i = a_i + b_i T + c_i T^2 \]  

(3.25)

In the above relation temperature is in °K, \( \mu_i \) is in lbm of 1/ft-sec and the coefficients \( a_i, b_i, \) and \( c_i \) are given in Table 3.3. For a mixture consisting of \( n \) gaseous species viscosity was predicted by the Buddenberg-Wilke model (Ref. 3.5)

\[ \mu = \frac{\sum_i y_i \mu_i}{\sum_i y_i \phi_{ij}} \]  

(3.26)

where

\[ \phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-1/2} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2 \]  

(3.27)

and \( M_i \) is the \( i \)th species molecular weight.

**Thermal Conductivity**

The species thermal conductivities were obtained from linear fits of theoretical results:

\[ K_i = d_i + e_i T \]  

(3.28)

again \( T \) is in °K, \( K_i \) is in °K, \( K_i \) is in BTU/ft - sec - °R and the coefficients \( d_i \) and \( e_i \) are given in Table 3.4. Mixture thermal conductivity is compared by

\[ k = \sum_i y_i \frac{K_i}{\sum_i y_i \phi_{ij}} \]  

(3.29)

where as before \( \phi_{ij} \) is given by Eq. 3.27.

**Binary Diffusion**

The coefficient of binary diffusion was assumed to be a function of temperature and pressure as follows (Ref. 3.4):

\[ D = \frac{8.128 \times 10^{-8} T^{1.659}}{P} \]  

(3.30)
TABLE 3.3

CONSTANTS FOR VISCOSITY CORRELATION

\[ \mu_i = a_i + b_iT + c_iT^2 \text{ lbm ft-sec} \]

<table>
<thead>
<tr>
<th>Species</th>
<th>( a \times 10^5 )</th>
<th>( b \times 10^7 )</th>
<th>( c \times 10^{12} )</th>
<th>Temperature Range (°K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( O_2 )</td>
<td>1.693</td>
<td>0.1496</td>
<td>-0.2276</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( N_2 )</td>
<td>0.970</td>
<td>0.1613</td>
<td>-0.1916</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( O )</td>
<td>1.519</td>
<td>0.1875</td>
<td>-0.2228</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( N )</td>
<td>0.253</td>
<td>0.2206</td>
<td>-0.3737</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( O^+ )</td>
<td>0.0</td>
<td>0.0500</td>
<td>-0.1000</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( N^+ )</td>
<td>0.0</td>
<td>0.0500</td>
<td>-0.1000</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( e^- )</td>
<td>0.0</td>
<td>0.0500</td>
<td>-0.1000</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( C )</td>
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<td>0.1772</td>
<td>-0.3378</td>
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</tr>
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<td>( H )</td>
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<td>0.0889</td>
<td>-0.0811</td>
<td>4,000-10,000</td>
</tr>
<tr>
<td>( H_2 )</td>
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<td>0.0791</td>
<td>-0.0886</td>
<td>4,000-10,000</td>
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<tr>
<td>( CO )</td>
<td>2.404</td>
<td>0.1363</td>
<td>-0.2184</td>
<td>4,000 - 9,000</td>
</tr>
<tr>
<td>( C_3 )</td>
<td>2.019</td>
<td>0.1179</td>
<td>-0.1655</td>
<td>1,000 - 5,000</td>
</tr>
<tr>
<td>( CN )</td>
<td>2.404</td>
<td>0.1363</td>
<td>-0.2184</td>
<td>4,000 - 9,000</td>
</tr>
<tr>
<td>( C_2H )</td>
<td>2.404</td>
<td>0.1363</td>
<td>-0.2184</td>
<td>4,000 - 9,000</td>
</tr>
<tr>
<td>( C_2H_2 )</td>
<td>1.396</td>
<td>0.0842</td>
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<tr>
<td>( C_3H )</td>
<td>2.019</td>
<td>0.1179</td>
<td>-0.1655</td>
<td>1,000 - 5,000</td>
</tr>
<tr>
<td>( C_4H )</td>
<td>2.019</td>
<td>0.1179</td>
<td>-0.1655</td>
<td>1,000 - 5,000</td>
</tr>
<tr>
<td>( HCN )</td>
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</tr>
<tr>
<td>( C_2 )</td>
<td>1.931</td>
<td>0.1393</td>
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<td>4,000 - 9,000</td>
</tr>
<tr>
<td>( C^+ )</td>
<td>0.0</td>
<td>0.0500</td>
<td>-0.1000</td>
<td>8,000-15,000</td>
</tr>
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</table>
TABLE 3.4
CONSTANTS FOR THERMAL CONDUCTIVITY CORRELATION

\[ k_i = a_i + b_i T \text{ (BTU/ft-sec-\( \text{oK} \))} \]

<table>
<thead>
<tr>
<th>Species</th>
<th>( a \times 10^5 )</th>
<th>( b \times 10^8 )</th>
<th>Temperature Range (( \text{oK} ))</th>
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</thead>
<tbody>
<tr>
<td>( \text{O}_2 )</td>
<td>1.019</td>
<td>0.4901</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( \text{N}_2 )</td>
<td>0.654</td>
<td>0.6457</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( \text{O} )</td>
<td>1.250</td>
<td>0.7092</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( \text{N} )</td>
<td>1.281</td>
<td>0.8593</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( \text{O}^+ )</td>
<td>26.0</td>
<td>0.0</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( \text{N}^+ )</td>
<td>26.0</td>
<td>0.0</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( \text{e}^- )</td>
<td>26.0</td>
<td>0.0</td>
<td>8,000-15,000</td>
</tr>
<tr>
<td>( \text{C} )</td>
<td>2.506</td>
<td>0.7479</td>
<td>5,000-10,000</td>
</tr>
<tr>
<td>( \text{H} )</td>
<td>2.496</td>
<td>5.129</td>
<td>4,000-10,000</td>
</tr>
<tr>
<td>( \text{H}_2 )</td>
<td>3.211</td>
<td>5.344</td>
<td>4,000-10,000</td>
</tr>
<tr>
<td>( \text{CO} )</td>
<td>0.859</td>
<td>0.6233</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{C}_3 )</td>
<td>0.630</td>
<td>0.5804</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{CN} )</td>
<td>0.859</td>
<td>0.6233</td>
<td>2,000-10,000</td>
</tr>
<tr>
<td>( \text{C}_2\text{H} )</td>
<td>1.126</td>
<td>0.7439</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{C}_2\text{H}_2 )</td>
<td>1.126</td>
<td>0.7439</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{C}_3\text{H} )</td>
<td>0.630</td>
<td>0.5804</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{C}_4\text{H} )</td>
<td>0.630</td>
<td>0.5804</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{HCN} )</td>
<td>0.486</td>
<td>0.8714</td>
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</tr>
<tr>
<td>( \text{C}_2 )</td>
<td>0.859</td>
<td>0.6233</td>
<td>1,000-5,000</td>
</tr>
<tr>
<td>( \text{C}^+ )</td>
<td>26.0</td>
<td>0.0</td>
<td>8,000-15,000</td>
</tr>
</tbody>
</table>
where $T$ is in °K, $P$ is in atmospheres, and $D$ is in ft$^2$/sec.

**Chemical Kinetics**

Formulation of a kinetics model that describes the chemical reactions in the flow-field requires the investigation of innumerable possible reactions that can take place among the air and ablation product species that are present in the shock layer. Because of the complexity associated with kinetics models involving a large number of reactions only those reactions that are important may be considered. In other words, we seek to develop the simplest model capable of accurately describing the chemical kinetics of the flow-field.

Suppose that a number $m$ of chemical reactions of the form

$$
\sum_{i}^{n} v_{ij} S_i + \sum_{i}^{n} v_{ij}'' S_i \quad (j = 1, \ldots, m) \tag{3.31}
$$

where $n$ is the total number of species in the system, and $v_{ij}$ and $v_{ij}''$ are the stoichiometric coefficients of the reactants and products in the $j$th reaction, respectively, have been chosen as a kinetics model, then the rate of generation of species $i$ due to finite-rate chemical reactions ($\omega_i$) is given by the Law of Mass Action (Ref. 3.6) as

$$
\omega_i = \sum_{j=1}^{n} \left( v_{ij} - v_{ij}'' \right) f_j M_i \prod_{k=1}^{n} \left( \frac{\rho C_k}{M_k} \right) v_{k,j}^i
\tag{3.32}
$$

$$
- \sum_{j=1}^{n} \left( v_{ij} - v_{ij}'' \right) r_j M_i \prod_{k=1}^{n} \left( \frac{\rho C_k}{M_k} \right) v_{k,j}^i \quad (i = 1, \ldots, n)
$$

where $\rho$ is the density, $C_i$ is the $i$th species mass fraction, $M_i$ is the molecular weight of species $i$, and $f_j$ and $r_j$ are the forward and backward reaction rate constants for the $j$th reaction, respectively. The forward and backward reaction rate constants are generally taken as functions of temperature of the form (Ref. 3.7)

$$
f_j = a_{fj} T^{b_{fj}} \exp \left( -e_{fj}/T \right) \quad (j = 1, \ldots, m) \tag{3.33}
$$

$$
r_j = a_{rj} T^{b_{rj}} \exp \left( -e_{rj}/T \right) \quad (j = 1, \ldots, m) \tag{3.34}
$$
where $a_{fj} T_{bfj}$ and $a_{rj} T_{bfj}$ are the frequency factors, and $e_{fj}$ and $e_{rj}$ are the activation energies for the $j$th forward and backward reactions, respectively.

In practice, the forward reaction rate constant is normally measured experimentally while the backward reaction rate constant is obtained as follows: At equilibrium

$$
\left( v''_{ij} - v'_{ij} \right) f_j M_i \prod_{k=1}^n \left( \frac{\rho C_{ik}}{M_k} \right) ^{v_{kj}'} = \left( v''_{ij} - v'_{ij} \right) r_j M_i \prod_{k=1}^n \left( \frac{\rho C_{ik}}{M_k} \right) ^{v'_{kj}}
$$

or

$$
f_j = \prod_{k=1}^n \left( \frac{\rho C_{ik}}{M_k} \right) ^{v''_{kj} - v'_{kj}} \quad (j = 1, \ldots, m) \quad (3.36)
$$

The equilibrium constant for the $j$th reaction ($K_j$) is given by (Ref. 3.8)

$$
K_j = (RT)^{\frac{n}{M}} \prod_{k=1}^n \left( \frac{\rho C_{ik}}{M_k} \right) ^{v''_{kj} - v'_{kj}} \quad (j = 1, \ldots, m) \quad (3.37)
$$

where $R$ is the ideal gas constant. Substitution of Eq. 3.37 in Eq. 3.36 and solving for $r_j$ yields

$$
r_j = (RT)^{\frac{n}{M}} \prod_{k=1}^n \left( \frac{\rho C_{ik}}{M_k} \right) ^{v''_{kj} - v'_{kj}} f_j K_j^{-1} \quad (j = 1, \ldots, m) \quad (3.38)
$$

Therefore, knowing the forward reaction rate constant and the equilibrium constant the backward rate constant can be obtained from Eq. 3.38.

There are two methods commonly used to obtain the equilibrium constant of a reaction. The first method consists of computing the chemical equilibrium composition of the system for a range of different temperatures and using this data with Eq. 3.37 to compute the equilibrium constant for different values of temperature. This set of values of equilibrium constant versus temperature can be curve fit with
analytical expression for $K_j$

$$K_j = V_j \exp \left( \frac{\beta_j}{T} \right) \quad (j = 1, \ldots, m) \quad (3.39)$$

where $V_j$ and $\beta_j$ are constants. The second method consists of using the expression for the equilibrium constant obtained from thermodynamics (Ref. 3.9)

$$K_j = \exp \left( -\frac{\Delta F_j^o}{RT} \right) \quad (j = 1, \ldots, m) \quad (3.40)$$

where $\Delta F_j^o$ is the standard free energy for the $j$th reaction and is given by

$$\Delta F_j^o = \frac{n}{k} \left( v_j'' - v_j' \right) \frac{P^o}{k} \quad (j = 1, \ldots, m) \quad (3.41)$$

$$\frac{\Delta F_j}{RT} = B_{1,j} \left( 1 - \ln T \right) - \frac{B_{2,j}}{2} \frac{T}{T} - \frac{B_{3,j}}{6} \frac{T^2}{T} - \frac{B_{4,j}}{12} \frac{T^3}{T}$$

$$- \frac{B_{5,j}}{20} \frac{T^4}{T} - \frac{B_{6,j}}{T} - \frac{B_{7,j}}{j}$$

where

$$B_{k,j} = \frac{n}{k} \left( v_j'' - v_j' \right) A_{k,j} \quad (k = 1, \ldots, 7)$$

Therefore the equilibrium constant may be obtained from the species standard free energy expressions given in Tables 3.1 and 3.2. The first method has the advantage that when it is used the backward reaction rate constant has the same form as Eq. 3.34; this can be seen by eliminating $f_j$ and $K_j$ from Eq. 3.38 by substituting Eqs. 3.33 and 3.39 to yield

$$r_j = \frac{(RT) n}{k} \left( v_j'' - v_j' \right) a_{f_j} \frac{b_{f_j}}{V_j} \exp \left[ \frac{-(e_{f_j} + \beta_j)}{T} \right] \quad (3.42)$$

Comparing Eqs. 3.42 and 3.34 it is evident that

$$a_{r_j} = \frac{(RT) n}{k} \left( v_j'' - v_j' \right) a_{f_j}$$

$$b_{r_j} = b_{f_j} + \frac{n}{k} \left( v_j'' - v_j' \right)$$

$$e_{r_j} = e_{f_j} + \beta_j \quad (3.43)$$

The second method, on the other hand, does not yield an expression of
the form of Eq. 3.34 since \( \Delta F^\circ_j \) is a polynomial expression (see Eq. 3.4). The resulting expression is therefore cumbersome to use. On the other hand the second method has the advantage that \( K_j \) is readily obtained from the species standard free energy and does not require a routine for computing chemical equilibrium as does the first method.

Up until this point, this discussion has been limited to the case where the kinetics model was already determined; however, as will be shown below, establishing an appropriate kinetics model is not a simple task. Information has been collected over a period of years on the chemistry of the reactions of ablation products and air species, and this information is stored in the form of a computer implemented data management file which presently contains several thousand reactions. It was necessary to examine this extensive set of reactions to arrive at a listing of most probable reactions (Ref. 3.10). These probable reactions were selected involving 28 species. Currently, it is not possible to consider a solution of the conservation equations with this many species and reactions. Furthermore, rate data were not available for many of them. Therefore, this preliminary list was then reexamined for key reactions to represent the chemical system. The selection was based on the species anticipated to have the largest compositions and presumably, therefore, dominate the energy level of the system. These key reactions are given in Table 3.5. In Table 3.6 the previously omitted ablation product and combustion reactions are given. Shown in Table 3.7 are the additional air and hydrogen combustion reactions. The values of the coefficients \( a_{fj} \), \( b_{fj} \), and \( e_{fj} \) of the forward reaction rate constants (see Eq. 3.33) for the reactions in Table 3.5 are given in Table 3.8. The forward rate constants listed
TABLE 3.5
SELECTED IMPORTANT CHEMICAL REACTIONS IN
THE SHOCK LAYER OF AN ABLATING BODY

1. \( \text{CO} + \text{N} = \text{CN} + \text{O} \)
2. \( \text{C}_2\text{H} + \text{H} = \text{C}_2 + \text{H}_2 \)
3. \( \text{N}_2 + \text{M} = 2\text{N} + \text{M} \)
4. \( \text{H}_2 + \text{M} = 2\text{H} + \text{M} \)
5. \( \text{O} + \text{M} = \text{O}^\cdot + \text{E}^- + \text{M} \)
6. \( \text{N} + \text{M} = \text{N}^\cdot + \text{E}^- + \text{M} \)
7. \( \text{CN} + \text{M} = \text{C} + \text{N}^\cdot + \text{M} \)
8. \( \text{CHN} + \text{M} = \text{CN} + \text{H} + \text{M} \)
9. \( \text{C}_2\text{H} + \text{M} = \text{C}_2 + \text{H} + \text{M} \)
10. \( \text{C}_2\text{H}_2 + \text{M} = \text{C}_2\text{H} + \text{H} + \text{M} \)
11. \( \text{CO} + \text{M} = \text{C} + \text{O} + \text{M} \)
12. \( \text{C}_3 + \text{M} = \text{C}_2 + \text{C} + \text{M} \)
13. \( \text{C}_2 + \text{M} = 2\text{C} + \text{M} \)
14. \( \text{C} + \text{M} = \text{C}^\cdot + \text{E}^- + \text{M} \)
15. \( \text{C}_3\text{H} + \text{M} = \text{C}_2\text{H} + \text{C} + \text{M} \)
16. \( \text{C}_4\text{H} + \text{M} = \text{C}_3\text{H} + \text{C} + \text{M} \)
### Table 3.6 Additional Ablation Product and Combustion Reactions

<table>
<thead>
<tr>
<th>CH₄, CH₃, CH₂, CH Reactions</th>
<th>C₂H₂, C₂H, Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CH₄ = CH₃ + H</td>
<td>1. C₂H₂ + H = C₂H + H₂</td>
</tr>
<tr>
<td>2. CH₄ = CH₂ + H₂</td>
<td>2. C₂H₂ + O = CH₂ + CO</td>
</tr>
<tr>
<td>3. CH₃ = CH₂ + H</td>
<td>3. C₂H₂ + OH = C₂H + H₂O</td>
</tr>
<tr>
<td>4. CH₂ = CH + H</td>
<td>4. C₂H + H = C₂ + H₂</td>
</tr>
<tr>
<td>5. CH₂ + H = CH + H₂</td>
<td>5. C₂H + O = CH + CO</td>
</tr>
<tr>
<td>6. CH = C + H</td>
<td>Other Reactions</td>
</tr>
<tr>
<td>7. C + H₂ = CH + H</td>
<td>1. C₂ + H = C + CH</td>
</tr>
<tr>
<td>8. CH₂ + O = CO + H₂</td>
<td></td>
</tr>
</tbody>
</table>

**CN Reactions**

1. 2CN = C₂ + N₂
2. CN + O = N + CO
**Table 3.7  Additional Air and Hydrogen Combustion Reactions**

<table>
<thead>
<tr>
<th>Air Reactions</th>
<th>Hydrogen Combustion Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ( \text{O}_2 + M = 20 + M )</td>
<td>1. ( H + \text{O}_2 = \text{OH} + O )</td>
</tr>
<tr>
<td>2. ( \text{N}_2 + M = \text{N}^+ + e^- + M )</td>
<td>2. ( O + \text{H}_2 = \text{OH} + H )</td>
</tr>
<tr>
<td>3. ( \text{NO} + M = \text{N} + \text{O} + M )</td>
<td>3. ( \text{OH} + \text{H}_2 = \text{H}_2\text{O} + H )</td>
</tr>
<tr>
<td>4. ( \text{NO} + O = \text{O}_2 + \text{N} )</td>
<td>4. ( 2\text{OH} = \text{H}_2\text{O} + O )</td>
</tr>
<tr>
<td>5. ( \text{N}_2 + \text{O} = \text{NO} + \text{N} )</td>
<td>5. ( H + \text{OH} + M = \text{H}_2\text{O} + M )</td>
</tr>
<tr>
<td>6. ( \text{N} + O = \text{NO}^+ + e^- )</td>
<td>6. ( H + O + M = \text{OH} + M )</td>
</tr>
</tbody>
</table>
TABLE 3.8 COEFFICIENTS OF THE
FORWARD REACTION RATE CONSTANTS

<table>
<thead>
<tr>
<th>jth Reaction</th>
<th>$a_{fj}$</th>
<th>$b_{fj}$</th>
<th>$e_{fj}$</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.0 E 18</td>
<td>.5</td>
<td>71,000</td>
<td>*</td>
</tr>
<tr>
<td>2</td>
<td>4.5 E 11</td>
<td>.5</td>
<td>35,000</td>
<td>Ref. 3.11</td>
</tr>
<tr>
<td>3</td>
<td>1.0 E 21</td>
<td>-1.5</td>
<td>224,900</td>
<td>3.12</td>
</tr>
<tr>
<td>4</td>
<td>3.6 E 18</td>
<td>-.82</td>
<td>103,000</td>
<td>3.13</td>
</tr>
<tr>
<td>5</td>
<td>2.8 E 12</td>
<td>.5</td>
<td>313,000</td>
<td>3.13</td>
</tr>
<tr>
<td>6</td>
<td>2.9 E 12</td>
<td>.5</td>
<td>333,000</td>
<td>3.13</td>
</tr>
<tr>
<td>7</td>
<td>2.2 E 20</td>
<td>-1.0</td>
<td>131,800</td>
<td>3.14</td>
</tr>
<tr>
<td>8</td>
<td>8.4 E 18</td>
<td>.5</td>
<td>120,000</td>
<td>*</td>
</tr>
<tr>
<td>9</td>
<td>9.5 E 18</td>
<td>.5</td>
<td>140,000</td>
<td>*</td>
</tr>
<tr>
<td>10</td>
<td>9.5 E 18</td>
<td>.5</td>
<td>117,000</td>
<td>*</td>
</tr>
<tr>
<td>11</td>
<td>8.5 E 19</td>
<td>-1.0</td>
<td>257,900</td>
<td>3.14</td>
</tr>
<tr>
<td>12</td>
<td>1.0 E 19</td>
<td>.5</td>
<td>190,000</td>
<td>*</td>
</tr>
<tr>
<td>13</td>
<td>9.3 E 18</td>
<td>.5</td>
<td>155,000</td>
<td>*</td>
</tr>
<tr>
<td>14</td>
<td>9.4 E 18</td>
<td>.5</td>
<td>265,000</td>
<td>*</td>
</tr>
<tr>
<td>15</td>
<td>9.5 E 18</td>
<td>.5</td>
<td>165,000</td>
<td>*</td>
</tr>
<tr>
<td>16</td>
<td>9.5 E 18</td>
<td>.5</td>
<td>145,000</td>
<td>*</td>
</tr>
</tbody>
</table>

\* Activation energy computed using the method described by Semenov (Ref. 3.15), and the frequency factor computed using collision theory (Ref. 3.16).
were the best experimental values or were computed theoretically. With these constants, \( R = 1.987 \text{ cal/gmole} - {^\circ}\text{K} \) and temperature in \( {^\circ}\text{K} \), the units of \( f_j \) are \( \text{cm}^3/\text{gm} - \text{mole} - \text{sec} \).

Originally the method proposed to obtain the equilibrium constants for the reactions in Table 3.5 was by a curve fit of equilibrium data. The chemical equilibrium composition for different values of temperature (from \( 1,000^\circ\text{K} \), to \( 15,000^\circ\text{K} \)) were computed with a free energy minimization chemical equilibrium program. This information was then used with Eq. 3.37 to obtain the value of the equilibrium constant for different temperatures. The results of this operation are shown in Fig. 3.1 for the reaction \( \text{C}_3\text{H}_6 \rightleftharpoons \text{C}_2\text{H} + \text{C} \) where \( \ln K \) is plotted versus \( 1/T \) (dotted line). These actual values of \( K \) were then least squares fit with an expression of the form of Eq. 3.39. The resulting analytical expression for \( K \) is also plotted in Fig. 3.1 (solid line). It can be seen that using the analytical expression for \( K \) instead of the actual values introduces significant error, for example at \( T = 10,000^\circ\text{K} \) the percentage error in \( K \) is 1000. This difficulty encountered in this reaction was found to be typical in some of the other reactions as well.

For this reason it was found more desirable to use the second method discussed above for obtaining \( K_j \). This was accomplished by obtaining \( \Delta F_j^\circ \) from Eq. 3.41 and then using Eq. 3.40 to obtain \( K_j \). Table 3.9 contains the values of the coefficients \( B_{1,j}, B_{2,j}, \ldots, B_{7,j} \) of Eq. 3.41 for the reactions in Table 3.5. The equilibrium constant \( K_j \) obtained, if plotted in Fig. 3.1, is undistinguishable from the curve of the actual values of \( K \).

**Radiative Properties**

The radiation flux divergence \( (dq_{R,y}/dy) \) appearing in Eq. 2.61
Figure 3.1 Equilibrium Constant and Its Linear Least Squares Fit. For the Reaction $C_3H \rightleftharpoons C_2H + C$
**TABLE 3.9**

**COEFFICIENTS OF THE EQUILIBRIUM CONSTANT CORRELATION**

<table>
<thead>
<tr>
<th>REACTION(*)</th>
<th>( B_{1,j} )</th>
<th>( B_{2,j} )</th>
<th>( B_{3,j} )</th>
<th>( B_{4,j} )</th>
<th>( B_{5,j} )</th>
<th>( B_{6,j} )</th>
<th>( B_{7,j} )</th>
<th>( T(**) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3530E+00</td>
<td>-0.7681E-03</td>
<td>0.5153E-06</td>
<td>-0.9618E-10</td>
<td>0.5427E-14</td>
<td>0.3485E+05</td>
<td>0.7500E-01</td>
<td>L</td>
</tr>
<tr>
<td></td>
<td>-0.9100E-01</td>
<td>0.2624E-03</td>
<td>0.8700E-09</td>
<td>0.5441E-11</td>
<td>0.2100E-15</td>
<td>0.4160E+05</td>
<td>0.2056E+01</td>
<td>H</td>
</tr>
<tr>
<td>2</td>
<td>0.1816E+01</td>
<td>-0.3571E-02</td>
<td>0.1634E-05</td>
<td>-0.2783E-09</td>
<td>0.1617E-13</td>
<td>0.1329E+05</td>
<td>0.8961E+01</td>
<td>L</td>
</tr>
<tr>
<td></td>
<td>-0.1852E+01</td>
<td>0.1831E-02</td>
<td>-0.5850E-06</td>
<td>0.7641E-10</td>
<td>-0.3417E-14</td>
<td>0.1329E+05</td>
<td>0.1126E+02</td>
<td>H</td>
</tr>
<tr>
<td>3</td>
<td>0.1727E+01</td>
<td>-0.8059E-03</td>
<td>0.1344E-06</td>
<td>-0.4980E-11</td>
<td>0.9780E-15</td>
<td>0.1132E+06</td>
<td>0.4274E+01</td>
<td>L</td>
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<tr>
<td></td>
<td>0.1765E+01</td>
<td>-0.1250E-02</td>
<td>0.3816E-06</td>
<td>-0.3536E-10</td>
<td>0.1003E-14</td>
<td>0.1132E+06</td>
<td>0.4450E+01</td>
<td>H</td>
</tr>
<tr>
<td>4</td>
<td>0.1642E+01</td>
<td>-0.2810E-03</td>
<td>0.9244E-07</td>
<td>-0.2914E-10</td>
<td>0.2112E-14</td>
<td>0.5196E+05</td>
<td>0.2626E+01</td>
<td>L</td>
</tr>
<tr>
<td></td>
<td>0.4505E+01</td>
<td>-0.4018E-02</td>
<td>0.1254E-05</td>
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<td>0.4213E-14</td>
<td>0.5196E+05</td>
<td>0.1348E+02</td>
<td>H</td>
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<tr>
<td>5</td>
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<td>0.1275E-10</td>
<td>-0.5056E-15</td>
<td>0.1580E+06</td>
<td>0.1181E+02</td>
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<td>0.2904E+01</td>
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<td>0.6591E-07</td>
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<td>0.1538E+02</td>
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</tr>
<tr>
<td>6</td>
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<td>-0.3726E-03</td>
<td>0.1864E-06</td>
<td>0.3765E-10</td>
<td>0.2271E-14</td>
<td>0.1686E+06</td>
<td>0.1238E+02</td>
<td>L</td>
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<tr>
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<td>0.2261E+01</td>
<td>0.3808E-03</td>
<td>0.1210E-06</td>
<td>0.1070E-10</td>
<td>0.3032E-15</td>
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<td>0.1003E+02</td>
<td>H</td>
</tr>
<tr>
<td>7</td>
<td>0.1675E+01</td>
<td>-0.6017E-03</td>
<td>0.6914E-07</td>
<td>0.3996E-10</td>
<td>0.2991E-14</td>
<td>0.9406E+05</td>
<td>0.3698E+01</td>
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<td>0.1414E+01</td>
<td>-0.8027E-03</td>
<td>0.1697E-06</td>
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<td>0.3831E-15</td>
<td>0.8731E+05</td>
<td>0.5594E+01</td>
<td>H</td>
</tr>
<tr>
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<td>-0.2955E-02</td>
<td>0.1359E-05</td>
<td>0.2518E-09</td>
<td>0.1668E-13</td>
<td>0.5850E+05</td>
<td>0.1912E+01</td>
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</tr>
<tr>
<td></td>
<td>0.3753E+01</td>
<td>-0.4486E-02</td>
<td>0.1768E-05</td>
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<td>0.6819E+01</td>
<td>H</td>
</tr>
</tbody>
</table>

* SEE TABLE 3.5 FOR REACTIONS

** TEMPERATURE RANGE L = 1,000-6,000 DEG. K, H = 6,000-15,000 DEG. K
### TABLE 3.9

COEFFICIENTS OF THE EQUILIBRIUM CONSTANT CORRELATION (Continued)

<table>
<thead>
<tr>
<th>REACTION(*)</th>
<th>B₁,j</th>
<th>B₂,j</th>
<th>B₃,j</th>
<th>B₄,j</th>
<th>B₅,j</th>
<th>B₆,j</th>
<th>B₇,j</th>
<th>T(**)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>0.3458E+01-0.3852E-02</td>
<td>0.1541E-05-0.2492E-09</td>
<td>0.1406E-13</td>
<td>0.6525E+05-0.6335E+01</td>
<td>L</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.2653E+01-0.2187E-02</td>
<td>0.6688E-06-0.8277E-10</td>
<td>0.3596E-14</td>
<td>0.6525E+05-0.2220E+01</td>
<td>H</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.2094E+01-0.2155E-02</td>
<td>0.7206E-06-0.1067E-09</td>
<td>0.5735E-14</td>
<td>0.5766E+05-0.3671E+01</td>
<td>L</td>
<td></td>
<td></td>
<td></td>
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* SEE TABLE 3.5 FOR REACTIONS

** TEMPERATURE RANGE L = 1,000-6,000 DEG. K, H = 6,000-15,000 DEG. K
is defined as follows (see Eq. 2.14)

$$\frac{dq_{R,Y}}{dy} = - 2 \pi \int \alpha_v (2B_v - I_v) \, dv$$

(3.44)

where

- $q_{R,Y}$ = radiative flux in a direction normal to the body
- $\alpha_v$ = volumetric absorption coefficient,
- $B_v$ = Plankian radiation intensity,
- $I_v$ = spectral radiation intensity,
- $v$ = frequency

Radiative mechanisms in high temperature gases may be categorized into those which produce radiation of a given frequency and those which produce radiation over a wide spectrum. The first of these groups of mechanisms is known as a line radiation mechanism (results from electronic transition between the bound energy levels in atoms or molecules), while the second group are commonly referred to as continuum radiation mechanisms (transfer between ionic states for atomic and molecular species, and transitions between two free energy levels in which free electrons are present in both the initial and final states).

One consequence of the existence of line and continuum radiative mechanisms is that the volumetric absorption coefficient ($\alpha_v$) for a high temperature gas varies discontinuously with wavelength. This fact requires that the integration of Eq. 3.44 be carried out on a piecewise basis over the frequency domain. The frequency range is divided into regions (bands) within which the discontinuous variations are averaged. Continuum radiation bands are used to represent regions of continuous radiation while line radiation bands are used to model the effect of the various discontinuous contributions. As in the numerical
integration of continuous functions, the use of more bands (smaller intervals) leads to a more accurate representation of the radiative process.

The radiative model used in the present work was developed by Engel (Ref. 3.17) from a model originally developed by Wilson (Ref. 3.18). The computer program developed by Engel computes both the radiative flux \( q_{R,y} \), and the radiative flux divergence \( \frac{dq_{R,y}}{dy} \) for a mixture of air and ablation products. The model uses nine line frequency bands and twelve continuum bands. It considers the following species and radiation mechanisms:

- \( H \)
- \( O_2 \)
- \( CO \)
- \( C \) Line and \( N_2 \)
- \( C_3 \) Continuum
- \( O \) Continuum \( C_2 \)
- \( C_2H \)
- \( N \)
- \( H_2 \)

REFERENCES


CHAPTER 4

THE SOLUTION METHOD

The mathematical model of stagnation-line flow contains a series of assumptions designed to simplify the mathematics of the problem without significantly reducing the accuracy of the solution. However, the resulting equations are still non-linear, integral, and coupled and have variable coefficients, therefore an analytical solution cannot be obtained. This means that integration of the equations must be accomplished numerically. Before an attempt is made to formulate a numerical solution scheme, it is convenient to nondimensionalize and transform the equations of the stagnation line model (Table 2.9). After the model has been transformed, the behavior of specific terms, equations, and the entire system of equations will be investigated so that a solution method may be established. The solution method will then be implemented with a computer program.

NONDIMENSIONALIZATION AND TRANSFORMATION

Using the dimensionless variables given in Table 4.1, the stagnation line model can be written in the dimensionless form given in Table 4.2. Notice that the only difference between the dimensionless variables given in Table 4.1 and those used for the order of magnitude assessment in Chapter 2 (Table 2.2) is that in the former \( \rho_{\delta,0}^* \) is used in place of \( \rho_{\infty}^* \). This has the effect of introducing into the momentum equation (Eq. 4.2) a Reynolds Number based upon post-shock density as opposed to the free-stream...
TABLE 4.1

DIMENSIONLESS VARIABLES

\[
\begin{align*}
    u &= \frac{u^*}{U_\infty} \\
    v &= \frac{v^*}{U_\infty} \\
    \rho &= \frac{\rho^*}{\rho_{\delta,0}} \\
    T &= \frac{T^*}{T_{\delta,0}} \\
    C_p &= \frac{C_p^*}{2U_\infty} \\
    k &= \frac{k^*}{R^* \delta_{\delta,0} U_\infty^3} \\
    q_{R,y} &= \frac{q_{R,y}^*}{\rho_{\delta,0}^* U_\infty^3} \\
    \rho &= \frac{\rho^*}{\rho_{\delta,0}^*} \\
    x &= \frac{x^*}{R^*} \\
    y &= \frac{y^*}{R^*} \\
    h &= \frac{h^*}{\frac{1}{2} U_\infty^2} \\
    h_1 &= \frac{h_1^*}{\frac{1}{2} U_\infty^2} \\
    D &= \frac{D^*}{R^* U_\infty} \\
    \omega_i &= \frac{\omega_i^*}{R^* \delta_{\delta,0} U_\infty^3} \\
    \frac{R}{M_1} &= \frac{T_{\delta,0}^*}{U_\infty^2} \frac{R^*}{M_1^*} \\
    Re &= \frac{\rho_{\delta,0}^* U_\infty R^*}{\mu_{\delta,0}^*} \\
\end{align*}
\]
TABLE 4.2

DIMENSIONLESS STAGNATION LINE MODEL

EQUATIONS:

Species Continuity:

\[
\frac{d}{dy} \left( \rho \frac{dC_i}{dy} \right) - \rho v \frac{dC_i}{dy} + \omega_i = 0 \quad (i = 1, \ldots, n) \tag{4.1}
\]

X-momentum:

\[
\frac{1}{Re} \frac{d}{dy} \left( \frac{\frac{1}{\rho} \frac{d(\rho v)}{dy}}{dy} \right) - \rho v \frac{d}{dy} \left( \frac{\frac{1}{\rho} \frac{d(\rho v)}{dy}}{dy} \right) - \frac{1}{2} \rho \left( \frac{\frac{1}{\rho} \frac{d(\rho v)}{dy}}{dy} \right)^2 - 4 \rho (1 - \rho) \left( \frac{d\phi}{dx} \right)^2 = 0 \tag{4.2}
\]

Energy:

\[
\frac{2k}{c_p} \frac{d^2h}{dy^2} + \left[ - \rho v + \frac{d(C_p)}{dy} \right] \frac{dh}{dy} = \frac{2dR_y}{dy} \tag{4.3}
\]

Caloric Equation of state:

\[
h = \sum_{i}^{n} C_i h_i (T) \tag{4.4}
\]
TABLE 4.2 (CONTINUED)

Thermal Equation of State:

\[ \rho \cdot R \cdot T \left( \sum_{i} \frac{P_{i}}{M_{i}} \right) = P_{\delta} \] \hspace{1cm} (4.5)

Boundary Conditions:

Wall \((y = 0)\)

1. \(\rho v = (\rho v)_{w}\)

2. \(\frac{d(\rho v)}{dy} = 0\)

3. \(C_{i} = C_{i,w} \quad (i = 1, \ldots, n)\)

4. \(h = h_{w}\)

Shock \((y = \delta)\)

1. \(\rho v = (\rho v)_{\delta} = v_{\delta}\)

2. \(\frac{d(\rho v)}{dy} = -2 \left( \frac{\partial u_{\delta}}{\partial x} \right)_{x = 0}\)

(4.6)

3. \(C_{i} = C_{i,\delta} \quad (i = 1, \ldots, n)\)

4. \(h = h_{\delta}\)
Reynolds number previously used.

The mathematical model, as originally developed in Chapter 2 (Table 2.9), included the energy equation in temperature form (Eq. 2.61). During the present investigation the early attempts at solving the model concentrated on this formulation. However, after much computational experimentation led consistently to failure, it was decided to try a different formulation of the energy equation. The energy equation in terms of dimensionless temperature

\[ \frac{dT}{dy} - \frac{1}{2} \rho v C_p \frac{dT}{dy} + \frac{1}{2} \frac{d}{dy} \left[ \rho D \left( \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \left( h_i \frac{\partial C_i}{\partial y} \right) \right) \right] \]

\[ - \rho v \frac{d}{dy} \left( \frac{\partial}{\partial y} \left( h_i \frac{\partial C_i}{\partial y} \right) \right) - \frac{d}{dy} \left( \begin{array}{l} \rho D \left( \frac{\partial}{\partial y} \left( H_i \right) \right) \end{array} \right) = 0 \]

was transformed to an enthalpy form by nondimensionalizing Eq. 2.60 to yield

\[ \frac{dT}{dy} = \frac{1}{C_p} \frac{dh}{dy} - \frac{1}{C_p} \sum_{i=1}^{n} h_i \frac{dC_i}{dy} \]

and substituting Eq. 4.3b in Eq. 4.3a to yield Eq. 4.3 (see Table 4.2).

The model with the temperature form of the energy equation consisted of 3 + n equations in the unknowns \( \rho, v, T \) and \( C_i \) (\( i = 1, \ldots, n \)). The modified model includes the enthalpy as an additional unknown (temperature continues to be an unknown since the thermodynamic, transport, radiative, and chemical kinetics properties are explicit function of \( T \)), and therefore requires an additional equation. This equation is the caloric equation of state (Eq. 4.4). The boundary conditions on the energy equation are now \( h = h_0 \) at \( y = 0 \) and \( h = h_0 \) at \( y = 6 \).

The equations given in Table 4.2 can now be transformed using the Dorodnitsyn transformation defined as:
\[ \eta = \frac{\int_0^y \rho \, dy}{\int_0^y \rho \, dy} = \frac{\int_0^y \delta \, dy}{\int_0^y \delta \, dy} \quad (4.7) \]

From the above equation,

\[ \frac{d}{dy} = \frac{\rho}{\delta} \frac{d}{dn} \quad (4.8) \]

and this relation yields the equations given in Table 4.3. Notice that the Dorodnitsyn transformation converts the independent variable \( y \) to the new independent variable \( \eta \). Before proceeding to discuss the numerical solution to Eqs. 4.9 - 4.11 and Eqs. 4.4 and 4.5 it is convenient to rewrite the equations in a form more suitable for numerical solution.

Species continuity:

Expanding the second order term in Eq. 4.9 and rearranging gives

\[ \rho^2 \frac{D}{dn^2} \frac{\partial^2 C_i}{\partial \eta^2} + \left[ \frac{d(\rho D)}{dn} - \delta \rho v \right] \frac{\partial C_i}{\partial \eta} + \frac{\delta}{\rho} \omega_i = 0 \quad (i = 1, \ldots, n) \quad (4.13) \]

X-momentum:

Let us define a new dependent variable as follows

\[ f = \frac{\rho v}{(\frac{d(v)}{dn})_{\eta = 1}} \quad (4.14) \]

therefore

\[ \frac{df}{dn} = \frac{\frac{d(v)}{dn}}{\left(\frac{d(v)}{dn}\right)_{\eta = 1}} \quad (4.15) \]

When the global continuity equation is nondimensionalized and transformed into \( \eta \)-space the result is

\[ 2 \left(\frac{\partial u}{\partial x}\right)_{x = 0} = \frac{1}{\delta} \frac{d(v)}{dn} \quad (4.16) \]
TABLE 4.3
TRANSFORMED STAGNATION LINE MODEL

EQUATIONS:

Species Continuity:

\[
\frac{d}{dn} \left( \frac{\rho^2}{\delta} \frac{dC_i}{dn} \right) - \delta \rho v \frac{dC_i}{dn} - \frac{\delta^2}{\rho} \omega_i = 0 \quad (i = 1, \ldots, n)
\]  
(4.9)

X-momentum:

\[
\frac{d}{dn} \left( \frac{d^2(\rho v)}{dn^2} \right) - \delta R_v \rho v \frac{d^2(\rho v)}{dn^2} - 4\delta R_v \rho (1-\rho) \frac{d^2}{d\xi} \frac{d\phi}{dx} = 0
\]  
(4.10)

Energy:

\[
\frac{2}{\delta} \frac{\rho k}{C_p} \frac{d^2h}{dn^2} + \left[ -\rho v + \frac{1}{\delta} \frac{d}{dn} \left( 2\rho k \right) \right] \frac{dh}{dn} = 0
\]  
(4.11)

\[
2 \frac{\delta}{\rho} \frac{dq_{R_g}}{dy} + 2\rho v \frac{dv}{dn} + \frac{1}{\delta} \frac{d}{dn} \left( \frac{2\rho k}{C_p} - \rho^2 D \right) \frac{h_i}{H_i} \frac{dC_i}{dn} = 0
\]

Caloric Equation of State:

\[
h = \frac{\rho}{H_i} C_i H_i
\]  
(4.4)
TABLE 4.3 (CONTINUED)

Thermal Equation of State:

\[ \rho \, R \, T \left( \frac{C_i}{M_i} \right) = P_\delta \]  \hspace{1cm} (4.5)

Boundary Conditions:

Wall \((\eta = 0)\) \hspace{3.5cm} \text{Shock \((\eta = 1)\)}

1. \( \rho v = (\rho v)_w \)

2. \( \frac{d(\rho v)}{d\eta} = 0 \)

3. \( C_i = C_{i,w} \quad (i = 1, \ldots, n) \)

4. \( h = h_w \)

1. \( \rho v = (\rho v)_\delta = v_\delta \)

2. \( \frac{d(\rho v)}{d\eta} = -2\delta \left( \frac{\partial u_\delta}{\partial x} \right)_{x = 0} \)

3. \( C_i = C_{i,\delta} \quad (i = 1, \ldots, n) \)

4. \( h = h_\delta \)
Substitution of Eq.' 4.16 in Eqs. 4.14 and 4.15 gives

\[ f = - \frac{\rho v}{2 \delta} \frac{\partial u_\delta}{\partial x} \]  
(4.17)

\[ \frac{df}{dn} = \frac{(\partial u_{\delta x})_{x = 0}}{(\partial x)_{x = 0}} \]  
(4.18)

Making use of L'Hopital's rule,

\[ \lim_{x \to 0} \frac{u}{u_\delta} = \frac{(\partial u_{\delta x})_{x = 0}}{(\partial x)_{x = 0}} \]  
(4.19)

and

\[ \frac{df}{dn} = \lim_{x \to 0} \frac{u}{u_\delta} \]  
(4.20)

follows from Eqs. 4.18 and 4.19.

Substitution of Eq. 4.17 in Eq. 4.10 gives

\[ \frac{d(\rho u_{\delta x})}{dn} + Re \delta \frac{2}{(\partial x)_{x = 0}} \left[ 2f \frac{df}{dn} - \left( \frac{df}{dn} \right)^2 \right] \]  
(4.21)

\[ + 2 \frac{\mu}{\rho} (1 - \rho) \frac{(\partial u_{\delta x})_{x = 0}}{(\partial x)_{x = 0}} = 0 \]

The boundary conditions for this equation are

Wall (\( \eta = 0 \)):

\[ \begin{align*}
1. f &= - \frac{\rho v}{2 \delta} \frac{\partial u_{\delta x}}{\partial x} \\
2. \frac{df}{dn} &= 0
\end{align*} \]

Shock (\( \eta = 1 \)):

\[ \begin{align*}
1. f &= - \frac{\nu_{\delta x}}{2 \delta} \frac{\partial u_{\delta x}}{\partial x} \\
2. \frac{df}{dn} &= 1
\end{align*} \]
The momentum equation, being third order, can be expanded into two coupled equations; one first order and the other second order by defining

\[ f = \frac{1}{\delta} \frac{df}{d\eta} \]  \hspace{1cm} (4.22)

and substituting into Eq. 4.21

\[ \rho u e_\delta \frac{d^2 z}{d\eta^2} + \left[ 2R e_\delta \frac{2\delta u_{e_\delta} \delta}{\partial x} \right] f + \left\{ d(\rho u) \right\} \frac{df}{d\eta} = 0 \]  \hspace{1cm} (4.23)

The resulting boundary conditions for Eqs. 4.22 and 4.23 are

Wall (\( \eta = 0 \)):

1. \( f = f_w = -\frac{(\rho u)w}{2\delta \frac{\partial u_{e_\delta} \delta}{\partial x}} \)

2. \( z = 0 \)

Shock (\( \eta = 1 \)):

1. \( f = f_\delta = -\frac{v\delta}{2\delta \frac{\partial u_{e_\delta} \delta}{\partial x}} \)

2. \( z = 1/\delta \)

As was discussed in Chapter 2, four boundary conditions need to be satisfied by the \( x \)-momentum equation, three because the equation is third order and the other since the shock stand-off distance (\( \delta \)) is unknown.

In terms of Eqs. 4.22 and 4.23, this means that these equations must satisfy all four of Eqs. 4.24. This is done in practice by applying the two boundary conditions on \( z \) and \( f \) shown above to Eqs. 4.23 and 4.22, respectively. Integration of Eq. 4.22 gives

\[ f = \frac{\delta}{\eta} \int_0^\eta z \, d\eta + f_w \]  \hspace{1cm} (4.25)

Evaluating this relation at \( \eta = 1 \) and solving for \( \delta \) yields

\[ \delta = \frac{f \delta - f_w}{\int_0^1 z \, d\eta} \]  \hspace{1cm} (4.26)
It is easily seen that substitution of Eqs. 4.25 and 4.26 in Eq. 4.23 yields a second order, non-linear, integro-differential equation with \( \delta \) as the only dependent variable (assuming that \( \rho(\eta) \) and \( \mu(\eta) \) are known). This equation can be solved for \( \delta \) and then Eq. 4.25 is used to complete the solution to the problem. An alternative method of solution used in the present work is iteration: guess a value of \( \delta \) and solve Eqs. 4.23 and 4.25 for \( f \) and \( \delta \), use the computed \( \delta \) in Eq. 4.26 to obtain a new value of \( \delta \) and repeat the above procedure using the new value of \( \delta \) as guess until the guessed and computed values of \( \delta \) are equal.

**Energy:**

Expansion of the second term on the right-hand side of Eq. 4.11 gives

\[
\frac{1}{\delta} \frac{d}{d\eta} \left[ \frac{2\rho k}{C_p} - \rho \frac{\partial^2 D}{\partial \eta^2} \right] \left( \frac{\partial h_i}{\partial \eta} \right) = \frac{1}{\delta} \frac{d}{d\eta} \left[ \frac{2\rho k}{C_p} - \rho \frac{\partial^2 D}{\partial \eta^2} \right] \left( \frac{n}{\sum_i h_i} \frac{dC_i}{d\eta} \right)
\]

or

\[
\frac{2 \rho k}{\delta C_p} \frac{d^2 h}{d\eta^2} + \left[ -\rho v + \frac{1}{\delta} \frac{d}{d\eta} \left( \frac{2\rho k}{C_p} \right) \right] \frac{d h}{d\eta} = 0
\]

or

\[
\frac{2 \delta}{\rho} \frac{d^2 q_{R, y}}{dy^2} + 2 \rho v^2 \frac{dv}{d\eta} + \frac{1}{\delta} \frac{d}{d\eta} \left[ \frac{2\rho k}{C_p} - \rho \frac{\partial^2 D}{\partial \eta^2} \right] \left( \frac{n}{\sum_i h_i} \frac{dC_i}{d\eta} \right)
\]

A summary of the dimensionless transformed equations is given in Table 4.4.

**METHODS OF COMPUTING REACTING FLOWS**

Historically the first attempts at solving the finite-rate chemistry
### TABLE 4.4

**SUMMARY OF DIMENSIONLESS TRANSFORMED EQUATIONS**

**EQUATIONS:**

**Species Continuity:**

\[ \rho^{2D} \frac{d^2C_i}{d\eta^2} + \left[ \frac{d(\rho^{2D})}{d\eta} - \delta \rho' v \right] \frac{dC_i}{d\eta} + \frac{\delta^2}{\rho} \omega_i = 0 \quad (i = 1, \ldots, n) \]  \hspace{1cm} (4.13)

**X-Momentum:**

\[ f = - \frac{\rho v}{2\delta} \frac{\partial u_{\delta,0}}{\partial x} \]  \hspace{1cm} (4.17)

\[ \rho \mu \frac{d^2z}{d\eta^2} + \left[ 2R_e \delta \frac{\partial u_{\delta,0}}{\partial x} \right] f + \frac{d(\rho u)}{d\eta} \frac{dz}{d\eta} \]  \hspace{1cm} (4.23)

\[ -R_e \delta \frac{\partial u_{\delta,0}}{\partial x} \frac{dz}{\partial x} + 2R_e \delta \frac{\rho}{\rho} (1 - \delta) \frac{d\phi}{dx} \frac{dz}{dx} = 0 = 0 \]

\[ f = \delta \frac{\partial u_{\delta,0}}{\partial x} \frac{dz}{dx} + f_w \]  \hspace{1cm} (4.25)

\[ \delta = \frac{f \delta - f_w}{f_1 \frac{dz}{d\eta}} \]  \hspace{1cm} (4.26)
TABLE 4.4 (CONTINUED)

Energy:

\[ \frac{2 \rho k}{C_p} \frac{d^2 h}{dn^2} + \left[ -\rho v + \frac{1}{\delta} \frac{d}{dn} \left( \frac{2\rho k}{C_p} \right) \right] \frac{dh}{dn} = \]

\[ \frac{2\delta}{\rho} \frac{dq_{R,v}}{dy} + 2\rho v \frac{dv}{dn} + \frac{1}{\delta} \frac{d}{dn} \left( \frac{2\rho k}{C_p} - \rho \gamma D \right) \frac{n}{\sum_i h_i} \frac{dc_i}{dn} \]

\[ + \frac{1}{\delta} \frac{2\rho k}{C_p} - \rho \gamma D \right) \frac{n}{\sum_i h_i} \frac{dh_i}{dn} \frac{dc_i}{dn} \]

\[ + \frac{1}{\delta} \left( \frac{2\rho k}{C_p} - \rho \gamma D \right) \frac{n}{\sum_i h_i} \frac{dc_i}{dn} \] (4.28)

Caloric Equation of State:

\[ h = \sum_i C_i h_i \] (4.4)

Thermal Equation of State:

\[ \rho \left( \frac{n}{\sum_i h_i} \right) \frac{C_i}{M_i} = P \delta \] (4.5)
problem were concentrated upon one-dimensional flows with no diffusion. The equations describing this physical situation are of the following form:

\[ \frac{dy_i}{dt} = f_i(y_1, y_2, \ldots, y_n) \quad (i = 1, 2, \ldots, n) \tag{4.29} \]

where the concentrations of species in an \( n \)-species system \((y_1, \ldots, y_n)\) are the dependent variables and time \((t)\) is the independent variable. These equations are non-linear, coupled through the right-hand-side term \((f_1, \ldots, f_n)\), and are subject to initial boundary conditions of the first kind. In attempting to numerically solve the above set of equations it was found that the classical integration techniques (Euler, Runge-Kutta, etc.) could be used to compute the solution for cases where the reaction rates were relatively slow, but for fast reaction rates (those occurring when the flow is near chemical equilibrium) the time required to integrate the equations became exorbitant. When the latter condition existed the equations were referred to as "stiff" equations by Curtiss and Hirschfelder (Ref. 4,1) because this type of problem arises also in overcontrolled servomechanical systems.

Numerical techniques for solving differential equations are generally judged on the basis of stability, accuracy, and speed of computation. Stability means that the numerical solution must follow the general form of the true solution. Accuracy measures how closely the numerical solution approximates the true solution. It should be clear that an algorithm may be stable but inaccurate. The computational speed depends upon the allowable stepsize and on the computational effort required to perform each step.
The solution of Eqs. 4.29 is normally carried out by locally linearizing the equations and solving at each step the resulting set of linear equations. The linearization is carried out by expanding each $f_i$ in a truncated Taylor series about a local point $t_m$ to yield

$$\frac{dy_i}{dt} = f_{i,m} + \sum_{j=1}^{n} \left( \frac{\partial f_i}{\partial y_j} \right)_m (y_j - y_{j,m}) \quad (i = 1, \ldots, n) \quad (4.30)$$

or

$$\frac{dy_i}{dt} = \sum_{j=1}^{n} A_{ij} y_j + B_i \quad (i = 1, \ldots, n) \quad (4.31)$$

where

$$A_{ij} = \left( \frac{\partial f_i}{\partial y_j} \right)_m \quad \text{and} \quad B_i = f_{i,m} - \sum_{j=1}^{n} \left( \frac{\partial f_i}{\partial y_j} \right)_m y_{j,m}$$

Equation 4.31 may be written as

$$\frac{dy}{dt} = A \bar{y} + B$$

using matrix notation where $\bar{y} = \begin{bmatrix} y_1, y_2, \ldots, y_n \end{bmatrix}^T$

$$B = \begin{bmatrix} B_1, B_2, \ldots, B_n \end{bmatrix}$$

and

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & \cdots & \frac{\partial f_2}{\partial y_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial y_1} & \frac{\partial f_n}{\partial y_2} & \cdots & \frac{\partial f_n}{\partial y_n} \end{bmatrix}$$

Techniques for solving Eq. 4.32 are generally classified as explicit, implicit and locally exact. Explicit techniques are those for which the values of each of the dependent variables at any step may be expressed explicitly in terms of the dependent variables at preceding steps. All
predictor-corrector methods, as well as all variants of the Runge-Kutta method are explicit. Implicit techniques are those for which the values of each of the variables at any step depends on itself and on the other dependent variables at that step as well as on the dependent variables at preceding steps. An implicit technique when applied to Eq. 4.32 always results in a set of linear algebraic simultaneous equations which must be solved for the vector $\tilde{y}$ at each step. Locally exact techniques solve Eq. 4.32 exactly to yield

$$y_i = \sum_{j=1}^{n} C_{ij} \tilde{y}_j \exp(\lambda_j h) + \tilde{y}_{i,p} \quad (i = 1, \ldots, n)$$

(4.33)

where the $C_{ij}$ are integration constants, the $\lambda_j$ are the eigenvalues of $\tilde{A}$, $h$ is the stepsize and $\tilde{y}_{i,p}$ are particular solutions to Eq. 4.32. This solution assumes that all the eigenvalues of $\tilde{A}$ are distinct.

All explicit techniques have finite stability boundaries, that is, they are stable for some stepsizes and unstable for others. Under conditions of stiffness, explicit techniques must use a very small stepsize in order to remain stable. On the other hand, they can be very accurate and require a modest degree of computational effort to compute a step. Some implicit techniques are unconditionally stable, in other words, the allowable stepsize is not restricted by stability requirements. However, their accuracy is generally limited and, because a set of linear algebraic equations must be solved, they require a fair amount of computational effort to perform a step. Locally exact methods are unconditionally stable and very accurate but, because the eigenvalues of $\tilde{A}$ must be computed for each step, require a large degree of computational effort to compute a step.

The numerical solution of stiff equations has been studied extensively and a number of techniques were proposed to cope with this problem.
Curtiss and Hirschfelder (Ref. 4.1) proposed an implicit technique for solving a single stiff equation. Emanuel (Ref. 4.2) studied the application of predictor-corrector and Runge-Kutta techniques to the chemical equations in near equilibrium flows. The locally exact method was applied by Moretti (Ref. 4.3) to the problem of combustion of hydrogen in air at constant pressure. He made a comparison of the computing time required using the locally exact method and the fourth order Runge-Kutta method.

Treanor (Ref. 4.5) developed an explicit method for solving non-linear stiff equations. It assumes that the basic equations can be approximated by a linearized form, but not the form given in Eqs. 4.30. Instead they are linearized as follows:

\[
\frac{d y_i}{dt} = -(P_i)_m y_i + (A_i)_m (i=1, \ldots, n) \quad \quad (4.34)
\]

\[
+ (B_i)_m h + (C_i)_m h^2
\]

where the \( P_i, A_i, B_i \) and \( C_i \) are constants in a given step but are allowed to vary from step to step.

Lomax and Bailey (Ref. 4.6) and Bailey (Ref. 4.12) studied the solution to the problem of air flow behind a normal shock by applying different numerical techniques. The techniques utilized were the explicit modified Euler method, the implicit modified Euler method and Treanor's method.

Magnus and Schechter (Ref. 4.15) developed a unified theory of numerical techniques based on rational approximations to the exponential terms in Eqs. 4.33. They showed that a number of explicit and implicit techniques are really rational approximations of different order. The
implicit methods studied, which include the method of collocation and the subdomain method, were shown to be unconditionally stable and the subdomain method was applied to the problems of hydrogen-air combustion and dissociating air.

From the work that has been carried out it has become evident that there is no "best" method for solving Eqs. 4.29. The optimum method to be used depends upon the degree of "stiffness" of the equations. If the flow is essentially frozen, classical explicit techniques such as fourth order Runge-Kutta are better than any implicit or locally exact method because they would be accurate and faster. If the flow is near chemical equilibrium, an unconditionally stable implicit technique is optimum because the stepsize would be restricted only by the truncation error. In general, the locally exact technique is less convenient than the explicit or implicit methods, but it yields more information about the system of equations.

This discussion has assumed that the problem represented by Eqs. 4.29 is "well behaved", this means that the solution is inherently stable, and our discussion of stability was centered around what is called induced instability, that is, instability induced by the numerical technique used. However, it can also happen that the problem is "ill posed" or inherently unstable (Ref. 4.16). This can happen, for example, when the general solution to Eqs. 4.29 contains exponentially growing terms which must be suppressed to fulfill the boundary conditions imposed on the problem. For example, the general solution to the equation

\[
\frac{dy}{dt} = y - t
\]

is given by

\[
y = C e^t + t + 1
\]
where $C$ is an integration constant. If the initial condition is given as $y(0) = 1$, which makes $C = 0$ so that the solution is a simple linear term growing only slowly in comparison with the exponential term, any numerical technique for solving Eq. 4.35 will introduce the exponential term into the computed solution resulting in inherent instability.

This type of condition is common in problems described by differential equations of the type

$$
D_i(x) \frac{d^2 y_i}{dx^2} + E_i(x) \frac{dy_i}{dx} = F_i(y_1, y_2, \ldots, y_n) \quad (i = 1, \ldots, n)
$$

(4.37)

where the $D_i$ and $E_i$ are functions of the independent variable $x$; the $F_i$ are nonlinear functions of $y_1, y_2, \ldots, y_n$, and Eqs. 4.37 are subject to the following boundary conditions

$$
y_i(0) = y_{i,0} \quad (i = 1, \ldots, n) \quad (4.38)
$$

$$
y_i(1) = y_{i,1} \quad (i = 1, \ldots, n) \quad (4.39)
$$

One physical situation described by Eqs. 4.37 - 4.39 is that arising from similar boundary layer flows including mass diffusion and finite-rate chemical reactions.

When the equations are inherently unstable the methods discussed above for solving Eqs. 4.29 are not effective. Such methods are usually referred to as "marching" techniques because the solution starts at one of the boundaries and, for each step taken, the solution marches towards the other boundary. When marching techniques are applied to a two-point boundary value problem, such as that represented by Eqs. 4.37 - 4.39, it is necessary to transform the problem into an initial value problem.
This is accomplished by guessing the value of the $\frac{dy_l}{dx}$ at $x = 0$ and using the marching technique to compute the $y_l$ at $x = 1$, if the computed $y_l$ at $x = 1$ differs from the desired values, it is necessary to iterate until the boundary conditions at $x = 1$ are met.

Because of the problems associated with the use of marching techniques, boundary layer flow problems including mass diffusion and finite-rate chemical reactions have been approached with what are known as "globally implicit" techniques. These are techniques which work directly with the two-point boundary value problem and produce in one step the solution over the domain of interest.

Fay and Kay (Ref. 4.16) used a globally implicit method to solve the equations describing a laminar, dissociating, nitrogen boundary layer at the stagnation point of an axisymmetric body. The boundary layer equations were first linearized about an initial trial solution (or previous iteration) in such a way that the equations are uncoupled (except implicitly through the trial solution). The equations were then cast into an implicit finite-difference form and solved in sequence, the trial solutions being updated after each solution had been obtained. This sequence of solutions was continued until the original differential equations were satisfied to the desired degree of accuracy.

Blottner (Ref. 4.17) studied techniques for solving the viscous shock layer flow at the stagnation point of a blunt body for air with finite-rate chemical reactions. He found that a globally implicit technique, such as the one used by Fay and Kay, produced converged solutions in a reasonable amount of time. Adams, et. al., (Ref. 4.18) applied the technique used by Fay and Kay to compute the inviscid and viscid flow fields around spherically blunted cone geometries, including injection of inert argon or chemically reacting carbon dioxide with chemical reactions
taking place at a finite-rate.

Liu (Ref. 4,19) studied the problem of hydrogen injection into air at an axisymmetric point including mass diffusion and non-equilibrium chemistry. He studied the applicability of various techniques, such as an implicit marching technique developed by Lomax (Ref. 4.10) and the globally implicit method used by Fay and Kay, and found that some of the methods could not be applied to the reacting flow problem and those that could be applied did not work for near chemical-equilibrium flows.

To be successful, any proposed solution method to the stagnation-line, finite-rate equations must be in accord with these previous studies.

**DECOUPLING THE EQUATIONS**

Although it is desirable to solve the equations in Table 4.4 in a coupled manner, practical considerations make it necessary to decouple them. It must be noticed that any attempt to solve the equations coupled would require the simultaneous solution of $7 + n$ (in our problem $n = 19$) non-linear, ordinary integro-differential and linear integral and algebraic equations.

An illustration of how coupled equations can be uncoupled is given by considering the problem of solving

\[
\frac{dL_1}{dt} = a_{11} L_1 + a_{12} L_2
\]  
\[
\frac{dL_2}{dt} = a_{21} L_1 + a_{22} L_2
\]

where $L_1$ and $L_2$ are the dependent variables and the $a_{ij}$'s are constants. If the function $L_2$ is guessed, $(L_2(0))$, then this value can be used in Eq. 4.40 to give

\[
\frac{dL_1}{dt}^{(1)} - a_{11} L_1^{(1)} = a_{12} L_2^{(0)}
\]
where $L_2^{(0)}$ is a known function of $t$. This equation can be solved for $L_1^{(1)}$ and this function can be used as a guess for $L_1$ in Eq. 4.41 to give

$$\frac{dL_2}{dt} - a_{22} L_2^{(1)} = a_{21} L_1^{(1)}$$

(4.43)

The function $L_2^{(1)}$ obtained from solving the equation above can then be compared to $L_2^{(0)}$; if they are equal the problem is solved, if not $L_2^{(1)}$ is used as the new $L_2^{(0)}$ and the procedure described above is repeated.

It is easy to see that the price that must be paid for reducing the original problem to that posed by Eqs. 4.42 and 4.43 is, in general, a greater amount of computation needed.

The scheme used to decouple the equations in Table 4.4 is given in Figure 4.1 while Table 4.5 contains the uncoupled equations. First of all, values of $\delta^{(0)}$, $\rho^{(0)}$, $(\rho u)^{(0)}$, and $C_{i}^{(0)}$ ($i = 1, \ldots, n$) are guessed.

With these functions it is possible to solve Eqs. 4.44 and 4.45 for $f^{(1)}$ and $\bar{z}^{(1)}$ (this section of the flowchart is that enclosed by the dotted lines), this is accomplished by guessing $f^{(0)}$ and solving Eq. 4.44 for $\bar{z}^{(1)}$, then Eq. 4.45 is solved for $f^{(1)}$. If $f^{(1)} = f^{(0)}$ we proceed to solve for $v^{(1)}$ and $\delta^{(1)}$, if not, $f^{(0)}$ and $f^{(1)}$ are used to compute the next guess $f^{(0)} = (1 - \lambda_1) f^{(0)} + \lambda_1 f^{(1)}$, where $0 < \lambda_1 < 1$ and the process is repeated. Once $f^{(1)}$ and $\bar{z}^{(1)}$ are known, Eqs. 4.46 and 4.47 are solved for $v^{(1)}$ and $\tilde{\delta}^{(1)}$, respectively. If $\tilde{\delta}^{(1)} = \tilde{\delta}^{(0)}$ the iterative process would stop, otherwise, the iterative process would continue.
Figure 4.1 Problem Flowchart

INPUT 
$\tilde{z}^{(0)}$, $\rho^{(0)}$, $(\rho \mu)^{(0)}$
$C_i(0)$ $(i = 1, \ldots, n)$

ITER = 0
ITER = ITER + 1

IS
ITER = 1?

No
INPUT f(0)

Yes

See Figure 4.2

SOLVE EQ. 4.44
FOR $Z^{(i)}$

A

SOLVE EQ. 4.45
FOR $f^{(i)}$

B

$f(0) = (1-\lambda_1)f(0) + \lambda_1 f(1)$

C

IS
$f(1) = f(0)$?

Yes

No
SOLVE EQ. 4.46 FOR $v$

SOLVE EQ. 4.47 FOR $\delta^0$

IS $\delta(l) = \delta(0)$?

Yes

$\delta(0) = (\delta(l) + \delta(0))/2$

D

OUTPUT RESULTS

END

SOLVE ENERGY EQ. (EQ. 4.48) AND CALORIC EQ. OF STATE (EQ. 4.50) FOR $h(l)$ AND $T(l)$

See Figure 4.3

SOLVE SPECIES EQ. (EQ. 4.49) AND THERMAL EQ. OF STATE (EQ. 4.50a) FOR $C_i(l)$ (i = 1, ..., n), AND $\rho(l)$

See Figure 4.4

COMPUTE $\mu^{(l)}$

$\phi(0) = \phi(l)$

$\rho(0) = \rho(l)$

$\rho(l) \mu^{(l)} (0) = \rho(l) \mu^{(l)} (1)$

$C(l) = C_i(l)$ (i = 1, ..., n)

G

Figure 4.1 Problem Flowchart (continued)
TABLE 4.5

DECOUPLED EQUATIONS

χ - Momentum

\[
\rho(0) \chi(0) \frac{d^2 \chi(1)}{d \eta^2} + \left[ 2 \operatorname{Re} \delta(0) \frac{\partial u_{\delta,0}}{\partial \chi} f(0) + \frac{d(\rho(0) \chi(0))}{d \eta} \right] \frac{d \chi(1)}{d \eta} = 0
\]

\[\tag{4.44}\]

\[- \operatorname{Re} \delta(0) \frac{3}{\rho(0)} \frac{\partial u_{\delta,0}}{\partial \chi} \chi(1)^2 + 2 \operatorname{Re} \delta(0) \frac{\rho(0)}{\rho(0)} (1 - \rho) \frac{d \phi}{d \chi} x = 0\]

\[\tag{4.44}\]

\[f(1) = \delta(0) \int_0^\eta \chi(1) d\eta + f_0\]

\[\tag{4.45}\]

\[v(1) = -2 \delta(0) \frac{\partial u_{\delta,0}}{\partial \chi} f(1)\]

\[\tag{4.46}\]

\[\delta(1) = \frac{f_0 - f_0}{1 - \int_0^\eta \chi(1) d\eta}\]

\[\tag{4.47}\]

Energy:

\[
\frac{2}{\delta(1)} \left( \frac{\partial k}{\partial \rho} \right) \left( \frac{d^2 h(1)}{d \eta^2} \right) + \left[ -\rho(0) v(1) + \frac{1}{\delta(1)} \frac{d \left( 2 p k \right)}{d \rho} \right] \frac{d h(1)}{d \eta} = 0
\]

\[\tag{4.48}\]

\[
\frac{2 \delta(1)}{\rho(0)} \frac{d q(0)}{d y} + 2p(0) \left( v(1)^2 \right) \frac{d v(1)}{d \eta} + \frac{1}{\delta(1)} \frac{d \left( 2 p k \right)}{d \rho} \frac{d h(1)}{d \eta} - \rho \frac{d^2 h(1)}{d \eta^2} = 0
\]

\[\tag{4.48}\]
TABLE 4.5 (Continued)

\[ + \frac{1}{\delta(1)} \left( \frac{2\rho k}{c_p} - \rho^2 D(0) \right) \left( \frac{\partial}{\partial n} \frac{d C_i}{d n} \right) + \frac{1}{\delta(1)} \left( \frac{2\rho k}{c_p} - \rho^2 D(0) \right) \]

\[ \left( \frac{n}{h_i} \frac{d^2 C_i}{d n^2} \right) \]

Species Continuity:

\[ \rho(0)^2 D(1) \frac{d^2 C_i(1)}{d n^2} + \left[ \frac{d(\rho(0)^2 D(1))}{d n} - \frac{\delta(1) \rho(0) v(1)}{\rho} \right] \frac{d C_i(1)}{d n} \]

\[ + \frac{\delta(1)^2}{\rho(0)} \omega^1(1) = 0 \quad (4.49) \]

Caloric Equation of State:

\[ T^1 = \text{fn} \{ h^1, C_1^0, \ldots, C_n^0 \} \quad (4.50) \]

Thermal Equation of State:

\[ \rho^1 = \frac{\rho}{\rho} = \frac{\rho}{\rho} \frac{C_i(1)}{T(1)} \quad (4.50a) \]
is ended and the results output, if not the values of $p^{(i)}$, $c_i^{(o)}$ ($i = 1, \ldots, n$), $v^{(1)}$ and $\delta^{(1)}$ are used in the energy equation (Eq. 4.48) to solve for $h^{(1)}$, and the caloric equation of state (Eq. 4.50) is solved for $T^{(1)}$. Then the species equation (Eq. 4.49) and the thermal equation of state (Eq. 4.50a) are solved for $c_i^{(1)}$ ($i = 1, \ldots, n$) and $\rho^{(1)}$. Once the temperature and concentration profiles are known, the new viscosity ($\mu^{(1)}$) is computed, and $\delta^{(1)}$, $\rho^{(1)}$, $(\rho\mu)^{(1)}$ and $c_i^{(1)}$ ($i = 1, \ldots, n$) can be used as guesses for the next iteration. The flowcharts for the operations noted in Figure 4.1 are given in Figures 4.2 - 4.4 to be developed below.

LINEARIZATION OF THE EQUATIONS

In the previous section the equations were decoupled (Table 4.5); this has the effect of making each equation independent from the rest except through the iterative process. However, the equations are still nonlinear with variable coefficients. In considering the kinds of numerical techniques that may be used to solve these equations, the fact that the boundary conditions are given on two different points in the flow-field suggests that "globally implicit" finite-difference approximations would be preferable to so-called "shooting" or "marching" techniques since the latter requires specifications of all boundary conditions on one point in the flow-field. As used in this work globally implicit means that each differential equation is substituted by finite-difference approximations over the entire flow-field, and this results in a set of simultaneous algebraic equations that when solved yield the value of the dependent variable at different points in the flow field. If this finite-difference technique is applied directly to the nonlinear equations the problem is reduced to solving a set of non-linear
algebraic equations; however, due to the present lack of efficient
techniques for solving sets of non-linear algebraic equations it is
more convenient to linearize the differential equations before they are
written in finite-difference form. When this is done the problem is
reduced to obtaining the solution to a set of linear algebraic equations,
a much easier problem.

Consider a non-linear ordinary differential equation of the form

\[ \frac{dL}{dt} = g(L, t) \tag{4.51} \]

where \( g(L, t) \) is the non-linear term. It is evident that there are var-
ious ways of linearizing this equation; the simplest one being to use
an approximation to the solution \( L^{(0)} \) to write

\[ \frac{dL^{(1)}}{dt} = g(L^{(0)}, t) \tag{4.25} \]

This equation is now linear since \( L^{(0)} \) is a known function of \( t \), it
may be solved for \( L^{(1)} \) and if \( L^{(1)} = L^{(0)} \) the answer has been found,
if not \( L^{(1)} \) is used as the new guess and the process is repeated. An­
other commonly used linearizing technique is to expand the non-linear
term in Eq. 4.51 about the function \( L^{(0)} \) in a Taylor series truncated
after the second term to yield

\[ g[L^{(1)}, t] = g[L^{(0)}, t] + \frac{\partial g[L^{(0)}, t]}{\partial t} (L^{(1)} - L^{(0)}) \tag{4.53} \]
and by substitution of this relation in Eq. 4.51

\[
\frac{dL^{(1)}}{dt} = \frac{\partial g}{\partial t} L^{(1)} = g \{L^{(1)}, t\} - \frac{\partial g}{\partial t} \{L^{(0)}, t\} L^{(0)} \tag{4.54}
\]

This technique is known as quasilinearization (Refs. 4.20 and 4.21), and has been used extensively to solve problems in fluid and orbital mechanics. It can be demonstrated that if the sequence \(\{L^{(K)}\}\) converges, that is if \(\lim_{K \to \infty} L^{(K)} = L\), it does it monotonically (for example if \(L^{(0)} < L\) for all \(t\) monotonicity of convergence means \(L^{(0)} < L^{(1)} \leq \ldots \leq L\), and quadratically

\[
\left| L^{(K+1)} - L^{(K)} \right| = N \left| L^{(K)} - L^{(K-1)} \right| \tag{4.55}
\]

where \(N\) is a constant. Although these two properties make the technique extremely powerful, in practice the computation of \(\partial g / \partial t\) may be very costly. Therefore, in some instances the simpler technique given by Eq. 4.52 may be preferable.

In the present application use will be made of both the simple linearization and quasilinearization techniques.

\(X\) - momentum!

The non-linear term in Eq. 4.44 is the \(Z^{(1)}^2\) term, and quasilinearization yields

\[
Z^{(1)}^2 = Z^{(0)}^2 + 2Z^{(0)} (Z^{(1)} - Z^{(0)})
\]

\[
= 2Z^{(0)} (Z^{(1)} - Z^{(0)})^2 \tag{4.56}
\]

when this relation is substituted in Eq. 4.44 the result is

\[
\frac{d^2 Z^{(1)}}{d \eta^2} + 2 \left[ \text{Re} \frac{\partial}{\partial \eta} \frac{\delta (\rho \mu) \theta}{\partial \eta} f(0) + \frac{d}{d \eta} \left( \frac{1}{\eta} \left( \rho^{(0)} \mu^{(0)} \right) \right) \right] \frac{dZ^{(1)}}{d \eta}
\]
This equation is now linear and may be solved as shown in Figure 4.2.

Energy:

The energy equation (Eq. 4.48) is linear in \( h^{(1)} \), and therefore linearization is not needed. Inversion of the caloric equation of state is accomplished as follows:

From Eq. 4.4

\[
\Delta T^{(k)} = \frac{h^{(1)} - \sum_{i}^{n} C_{i}^{(0)} h_{i}^{(k)}}{-\sum_{i}^{n} C_{i}^{(0)} C_{\rho i}^{(k)} (T^{(k)})}
\]

Since the \( h_{i}^{(k)} \) are nonlinear functions of \( T \), the Newton-Raphson technique was used:

\[
G^{(k)}(T) = h^{(1)} - \sum_{i}^{n} C_{i}^{(0)} h_{i}^{(k)}
\]

\[
T^{(k+1)} - T^{(k)} = -\frac{G^{(k)}(T^{(k)})}{\frac{dG}{dT}(T^{(k)})}
\]
Figure 4.2 Solution of X-momentum Equation

\[
Z^{(0)} = (1-\lambda_2)Z^{(0)} + \lambda_2 Z^{(1)}
\]
Using underrelaxation to obtain convergence

\[ T^{(k+1)} = T^{(k)} + \lambda_3 \Delta T^{(k)} \]

\[ = T^{(k)} + \lambda_3 \frac{h^{(1)} - h^{(k)}}{c_{p}^{(k)}} \quad 0 < \lambda_3 \leq 1 \] (4.58)

Once \( T^{(k+1)} \) has converged it becomes the new \( T^{(1)} \).

The flowchart for the solution of the equation of energy and the caloric equation of state for \( h^{(1)} \) and \( T^{(1)} \) is given in Fig. 4.3.

Species Continuity:

The reaction rate term in Eq. 4.49 is non-linear, therefore, quasilinearization gives

\[ \omega_i^{(1)} = \omega_i^{(0)} + \frac{\partial \omega_i^{(0)}}{\partial c_i} (c_i^{(1)} - c_i^{(0)}) \quad (i = 1, \ldots, n) \] (4.59)

and the species equation becomes

\[ \rho^{(0)} \frac{d}{d \eta} \left[ \frac{d^2 c_i^{(1)}}{d \eta^2} + \left[ \frac{d (\rho^{(0)})^2}{d \eta} \frac{D^{(1)}}{D} - \frac{\gamma^{(1)} \rho^{(0)}}{\rho^{(0)}} v^{(1)} \right] \frac{d c_i^{(1)}}{d \eta} \right] \]

\[ (i = 1, \ldots, n) \]

\[ + \frac{\omega_i^{(1)}}{\rho^{(0)}} \frac{\partial \omega_i^{(0)}}{\partial c_i} c_i^{(1)} = \frac{\gamma^{(1)}^2}{\rho^{(0)}} \left( \frac{\partial \omega_i^{(0)}}{\partial c_i} c_i^{(0)} - W_i^{(0)} \right) \] (4.60)

The scheme for solving the equation above and the thermal equation of state is given in Figure 4.4.

NUMERICAL SOLUTION OF THE EQUATIONS

As written in the previous section, the conservation equations (Eqs. 4.57, 4.58, and 4.60) are of the form
Solve Energy Equation (Eq. 4.48) for $h^{(1)}$

$h^{(0)} = (1-\lambda_4)h^{(0)} + \lambda_4 h^{(1)}$

Solve Caloric Equation of State (Eq. 4.58) for $T^{(1)}$

Figure 4.3 Solution of Energy Equation
Figure 4.4 Solution of Continuity Equation and Thermal Equation of State
\[ a_1 \frac{d^2 W}{d \eta^2} + a_2 \frac{dW}{d \eta} + a_3 W = a_4 \]  

(4.61)

where \( a_1, a_2, a_3, \) and \( a_4 \) are functions of \( \eta \). The numerical solution of Eq. 4.61 was accomplished by substituting finite-difference approximations for the derivatives in the equation. These approximations were obtained as follows: Knowing the value of \( W \) and its derivatives at any point \( \eta \) in the flow-field it is possible to write the Taylor series expression for the value of \( W \) at point \( \eta_{j-1} \)

\[ W_{j-1} = W_j + \frac{dW_1}{d \eta} (\eta_{j-1} - \eta_j) + \frac{d^2W_1}{d \eta^2} \left( \frac{\eta_{j-1} - \eta_j}{2} \right)^2 + 0 (\eta_{j-1} - \eta_j)^3 \]  

(4.62)

where \( W_j = W(\eta_j) \). Knowing \( W_j \) and its derivatives it is also possible to write an expression for \( W_{j+1} \)

\[ W_{j+1} = W_j + \frac{dW_{j+1}}{d \eta} (\eta_{j+1} - \eta_j) + 0 (\eta_{j+1} - \eta_j)^3 \]  

(4.63)

Neglecting higher order terms and solving Eqs. 4.62 and 4.63 first for \( \frac{dW_j}{d \eta} \) and then for \( \frac{d^2W_j}{d \eta^2} \) yields

\[ \frac{dW_1}{d \eta} \approx \frac{\Delta n_{j-1}}{\Delta n_j (\Delta n_j + \Delta n_{j-1})} W_{j+1} + \frac{\Delta n_{j-1} - \Delta n_{j-2}}{\Delta n_j \Delta n_{j-1}} W_j \]  

(4.64)

\[ + \frac{\Delta n_{j-1}}{\Delta n_{j-1} (\Delta n_j + \Delta n_{j-1})} W_{j-1} \]
\[
\frac{d^2 W_j}{d \eta^2} \propto \frac{2}{\Delta n_j (\Delta n_j + \Delta n_{j-1})} W_{j+1} + \frac{(-2)}{\Delta n_j \Delta n_{j-1}} W_j \\
+ \frac{2}{\Delta n_{j-1} (\Delta n_j + \Delta n_{j-1})} W_{j-1}
\]

(4.65)

where \( \Delta n_j = n_{j+1} - n_j \).

When Eq. 4.61 is evaluated at \( n_j \) and Eqs. 4.64 and 4.65 are introduced the result is

\[
\begin{bmatrix}
2\alpha_{1,j} - \Delta n_j \alpha_{2,j} \\
\Delta n_{j-1} (\Delta n_j + \Delta n_{j-1})
\end{bmatrix}
W_{j-1} + \begin{bmatrix}
-2\alpha_{1,j} + (\Delta n_j - \Delta n_{j-1}) \alpha_{2,j} \\
\Delta n_j \Delta n_{j-1}
\end{bmatrix}
W_j + \alpha_{3,j} = W_j
\]

\[
\begin{bmatrix}
2\alpha_{1,j} + \Delta n_{j-1} \alpha_{2,j} \\
\Delta n_j (\Delta n_j + \Delta n_{j-1})
\end{bmatrix}
W_{j+1} = \alpha_{4,j}
\]

(4.66)

Equation 4.66 is of the form

\[
A_j W_{j-1} + B_j W_j + C_j W_{j+1} = D_j
\]

(4.67)

Letting \( \eta_0 = 0 \) and \( \eta_m = 1 \) this means that \( W_0 \) and \( W_m \) are known since they are boundary conditions, when Eq. 4.67 is written for \( 1 \leq j \leq (m-1) \) the resulting set of equations is given in matrix notation by
The Thomas algorithm for tridiagonal matrices (Ref. 4.22) is a very efficient scheme for solving sets of linear algebraic equations involving tridiagonal matrices and has been used in this work to solve Eq. 4.68.

The solution of Equations (4.68) was accomplished by writing a computer program to perform the necessary calculations. This program (SLAC - Stagnation Line Analysis with Chemistry) includes the thermodynamic, transport, kinetic, and radiative properties discussed in Chapter 3, as well as, a subroutine to calculate local chemical equilibrium. The equilibrium calculation uses a free energy minimization technique developed by Del Valle and Pike (Ref. 4.23). SLAC is discussed in Appendix A and listed in Appendix B.

This program is a tool which models the stagnation region of an ablator-protected entry vehicle. Adequate boundary-conditions to describe the bow-shock and ablating surface, as described herein, must be specified to utilize this program.

REFERENCES


4.17 Blottner, F.G., "Viscous Shock Layer at the Stagnation Point with


CHAPTER 5
RESULTS OF STAGNATION REGION HEATING ANALYSIS

The SLAC program was used to compute the finite-rate and equilibrium-chemistry stagnation-line heating rate of a 9 foot entry vehicle moving at 50,000 feet/second when the free-stream air density is 8.85 x10^{-8} slugs/ft^3 and the mass injection rate \( \rho_w V_w / \rho_\infty U_\infty \) equals .05.

The vehicle is protected by a phenolic-nylon ablator with the following elemental composition (elemental mass fraction): 73.03% carbon, 7.29% hydrogen, 4.96% nitrogen and 14.72% oxygen. The char surface was assumed to be at the sublimation temperature of carbon at .1 atmosphere pressure (\( T_w = 3,450^\circ K \)). The shock was assumed to be concentric

\[ \frac{de}{dx} = 0, \quad \frac{d\phi}{dx} = 1. \]

These flight conditions and the rate of mass injection were used because they correspond to the conditions obtained by Engel (Ref. 5.1) when the ablator and the equilibrium shock layer solutions are coupled. In other words, according to his results, a vehicle moving under the flight conditions listed above and protected by phenolic-nylon ablates at a 5% rate. Furthermore, Esch (Ref. 5.2) also obtained chemical equilibrium results for the same flight conditions and injection rate. This means that the equilibrium results obtained during the present work may be compared to those obtained by the two investigators mentioned above. The comparison is more valid than in most cases since the same routine was used by all the investigators to solve the Rankine-Hugoniot equations. This means that the shock boundary conditions used were identical. In addition, the radiation model used was the same.
A complete solution to this entry-heating problem would admit nonequilibrium chemistry effects in the ablator response analysis. Such considerations could give different ablator species and (outside) wall temperatures. Even if the ablator effluent into the shock layer were in equilibrium, an entire new series of calculations similar to the ones done by Engel (Ref. 5.1) should be performed to determine the nonequilibrium coupled solution. Ablator non-equilibrium is not in the scope of this research, and non-equilibrium coupling must await the development of an adequate non-equilibrium shock layer analysis. This later development is precisely the subject of this research.

The wall and shock boundary conditions used in this study are given in Table 5.1. Table 5.2 presents a summary of the flight conditions used and the shock layer properties obtained. Since changes in flight conditions strongly affect the behavior of both chemical kinetics and shock layer calculations, the model and the solution scheme developed in this work should be studied over a wide range of flight conditions to determine its adequacy. In the present work only one set of flight conditions was considered, but it is believed that since the conditions are typical of those encountered during atmospheric entry, the model and its solution should work for a range of conditions similar to the ones considered.

**COMPUTATION OF BODY HEATING RATE**

Since computation of body heating rates for equilibrium and finite-rate chemistry was one of the stated objectives of this investigation, it is proper to discuss how this computation is performed.

As was discussed in Chapter 2, the stagnation line energy boundary condition at the body surface is given in dimensional form by
### TABLE 5.1 WALL AND SHOCK BOUNDARY CONDITIONS

<table>
<thead>
<tr>
<th></th>
<th>Wall (y = 0)</th>
<th>Shock (y = δ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ( \rho \dot{v} = 2.23 \times 10^{-4} \text{ slug ft}^{-2} \text{-sec} )</td>
<td>( \rho \dot{v} = -4.45 \times 10^{-4} \text{ slug ft}^{-2} \text{-sec} )</td>
<td></td>
</tr>
<tr>
<td>2. ( \frac{d(\rho v)}{dy} = 0 )</td>
<td>( \frac{d(\rho v)}{dy} = 8.5 \times 10^{-2} \text{ slug ft}^{-3} \text{-sec} )</td>
<td></td>
</tr>
<tr>
<td>3. ( T = 3,450^\circ \text{K} )</td>
<td>( T = 13,000^\circ \text{K} )</td>
<td></td>
</tr>
<tr>
<td>4. ( C_i ) = Chemical equilibrium composition of ablation products at 3,450(^\circ)K and 0.1 atmosphere</td>
<td>( C_i ) = Chemical equilibrium composition of air at 13,000(^\circ)K and 0.1 atmosphere</td>
<td></td>
</tr>
</tbody>
</table>
TABLE 5.2 SUMMARY OF FLIGHT CONDITIONS AND SHOCK LAYER PROPERTIES

\[ \rho_w = 8.85 \times 10^{-8} \text{ slug/ft}^3 \]
\[ U_w = 5 \times 10^4 \text{ ft/sec} \]
\[ \rho_w = 8.44 \times 10^{-6} \text{ slug/ft}^3 \]
\[ v_w = 2.64 \times 10^1 \text{ ft/sec} \]
\[ T_w = 3,450^\circ K \]
\[ \rho_\delta = 1.7 \times 10^{-6} \text{ slug/ft}^3 \]
\[ v_\delta = -2.62 \times 10^3 \text{ ft/sec} \]
\[ T_\delta = 13,000^\circ K \]
\[ \rho_\delta = 0.1 \text{ atm} \]
\[ \bar{\rho} = 0.0536 \]
\[ R = 9 \text{ ft} \]

Injection rate = 5%
\[
(\rho v H - k \frac{dT}{dy} + \sum_i n_i h_i j_{i,y} + q_{r,y})^+ = \\
(\rho v H - k \frac{dT}{dy} + \sum_i n_i h_i j_{i,y} + q_{r,y})^- = Q
\]

The heating rate \(Q\) is the net amount of energy heating the body. It must be recalled that the + and - superscripts refer to the shock layer and char sides of the interface, respectively. \(Q\) is computed by:

\[
Q = (\rho v H - k \frac{dT}{dy} + \sum_i n_i h_i j_{i,y} + q_{r,y})^+ 
\]

Preliminary calculations showed the first term in this equation to be negligible when compared to the other terms in the equation, for this reason it was not included in the computation of \(Q\). The heating rate to the body was expressed as

\[
Q = Q_c + Q_d + Q_R
\]

where

\[
Q_c = -k \frac{dT}{dy} = \text{Heat transfer by convection} 
\]

\[
Q_d = \sum_i n_i h_i j_{i,y} = \text{Heat transfer by diffusion} 
\]

\[
Q_R = q_{R,y} = \text{Heat transfer by radiation} 
\]

**FINITE-RATE CHEMISTRY RESULTS**

The SLAC program was used to compute non-equilibrium temperature, enthalpy, density, velocity and mass fractions profiles, and the body heating rate for the flight conditions previously discussed. Two sets of runs were performed, one using the chemical kinetics model described in Chapter 3, and the other using a modified kinetics model developed
by Balhoff (Ref. 5.3). The modified model assumes the same reactions used in the model described in Chapter 3, but the coefficients of the forward reaction rate constants were modified as shown in Table 5.3. Comparison of these coefficients to those in Table 3.8 shows that while the reactions used are the same, Balhoff's chemistry model uses significantly smaller reaction rate constants in 9 of the 16 reactions considered. Balhoff's model is in effect a modification of the original model used since it was found out that the frequency factors computed using collision theory were in error.

The results from both runs are presented here (Table 5.4) to give an indication of how sensitive the heating rate is to the value of the rate constants used. It must be pointed out that the solution using the rates in Table 5.3 were obtained in about 5% of the computer time, it took to obtain the solution with the original chemistry model (18 hours vs. 45 minutes in an IBM 360/65). This was probably due to the fact that the rates used in the original chemistry model were much faster than those in the modified model, and this made convergence of the species solution more difficult.

CHEMICAL EQUILIBRIUM RESULTS

Results obtained from the SLAC program using an equilibrium chemistry model for the flight conditions previously discussed provide profiles of temperature, enthalpy, density, velocity and mass fractions from the body surface ($y/\delta = 0$) to the shock ($y/\delta = 1$), and the body heating rate. It was maintained above that one of the reasons for choosing the flight conditions studied was the fact that both Engel (Ref. 5.1) and Esch (Ref. 5.2) had studied the same condition and, therefore, the validity of the equilibrium results obtained from SLAC
<table>
<thead>
<tr>
<th>jth Reaction</th>
<th>$a_{tj}$</th>
<th>$b_{fj}$</th>
<th>$c_{fj}$</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.09 E 10</td>
<td>0.5</td>
<td>71,000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4.50 E 11</td>
<td>0.5</td>
<td>35,000</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.10 E 21</td>
<td>-1.5</td>
<td>224,900</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3.60 E 18</td>
<td>-0.82</td>
<td>103,000</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2.80 E 12</td>
<td>0.5</td>
<td>313,000</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2.90 E 12</td>
<td>0.5</td>
<td>333,000</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>2.20 E 20</td>
<td>-1.0</td>
<td>131,800</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.09 E 10</td>
<td>0.5</td>
<td>120,000</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1.22 E 10</td>
<td>0.5</td>
<td>140,000</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.23 E 10</td>
<td>0.5</td>
<td>117,000</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>8.50 E 19</td>
<td>-1.0</td>
<td>257,900</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1.28 E 10</td>
<td>0.5</td>
<td>190,000</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>1.20 E 10</td>
<td>0.5</td>
<td>155,000</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1.21 E 10</td>
<td>0.5</td>
<td>165,000</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>1.09 E 10</td>
<td>0.5</td>
<td>115,000</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>1.09 E 10</td>
<td>0.5</td>
<td>145,000</td>
<td></td>
</tr>
</tbody>
</table>

*This rate constant is different from that used in the model described in Chapter 3.*
TABLE 5.4  NON-EQUILIBRIUM HEATING RATES AS PREDICTED BY TWO SETS OF RATE CONSTANTS

<table>
<thead>
<tr>
<th>Rate Constants</th>
<th>$Q_c$</th>
<th>$Q_d$</th>
<th>$Q_R$</th>
<th>$Q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 5.3</td>
<td>30</td>
<td>1</td>
<td>138</td>
<td>169</td>
</tr>
<tr>
<td>Table 3.8</td>
<td>4</td>
<td>1</td>
<td>106</td>
<td>111</td>
</tr>
</tbody>
</table>

*$\text{watts/cm}^2$*
could be corroborated.

Before proceeding to discuss and compare the results obtained to those obtained by Engel (Ref. 5.1) and Esch (Ref. 5.2), it is relevant to discuss the differences in the models used. Firstly, Engel used transport properties of air throughout the flow field (including the region from the stagnation point to the body) while Esch and the present work used properties of air and ablation products throughout the flow field. Secondly, the species wall boundary conditions are given by (See Eq. 2.50b).

$$\left( \rho v \right)_w C_{i,w} - J_{i,w} = \left( \rho v \right)_w C_{i}^- \quad (i = 1, \ldots, \eta)$$

(5.6)

where the term $J_i^-$, which corresponds to mass diffusion inside the char has been neglected, and the $C_i^-$ are the mass fractions obtained from the ablator response analysis. Esch assumed that mass diffusion could be described by using a binary diffusion coefficient $\left( J_i = -\rho D \frac{dC_i}{dy} \right)$, and used boundary conditions of the third kind:

$$\left( \rho v \right)_w C_{i,w} + \left( D \frac{dC_i}{dy} \right)_w = \left( \rho v \right)_w C_{i}^- \quad (i = 1, \ldots, \eta)$$

(5.7)

Engel assumed there was no diffusion throughout the flow field $\left( J_i(y) = J_{i,w} = 0 \right)$, and used boundary conditions of the first kind:

$$C_{i,w} = C_{i}^- \quad (i = 1, \ldots, \eta)$$

(5.8)

In the present investigation mass diffusion was allowed throughout the shock layer but, in order to simplify the solution to the species equations, the boundary conditions used at the wall were of the first kind:
Lastly, both Engel and Esch solved the energy equation in temperature form while in the present work an enthalpy form of the energy equation was used. As was discussed in Chapter 4, many attempts were made at solving the energy equation in temperature term, however, it was not possible to obtain a solution, and therefore, an enthalpy form of the equation was used.

The chemical equilibrium heating rates obtained by Engel, Esch and the present investigation are compared in Table 5.5. It must be noticed that Engel and Esch did not include the heat transfer to the body by diffusion.

The significant difference in convective heating rates, with the present investigation yielding an essentially negligible heating rate by convection, results because the present investigation predicts smaller temperature gradients near the wall than those predicted by Engel and Esch. In other words, the present investigation predicts a higher convective heating blockage effect resulting from injection of ablation products into the flow field.

**COMPARISON OF PREDICTED NON-EQUILIBRIUM AND EQUILIBRIUM HEATING RATES**

From the results shown in Tables 5.4 and 5.5 it is evident that the predicted equilibrium heating rate is approximately three times as large as the non-equilibrium heating rate, and for both cases most of the body heating is the result of radiation.

The lower radiative heating rate predicted by the non-equilibrium computation may be explained by examining the changes in chemical composition which occur in the shock layer. When the chemical compositions predicted by the equilibrium and the non-equilibrium calculations are
### Table 5.5 Equilibrium Heating Rates Obtained by Different Investigators

<table>
<thead>
<tr>
<th>INVESTIGATOR</th>
<th>$Q_{c}$</th>
<th>$Q_{d}$</th>
<th>$Q_{R}$</th>
<th>$Q^{*}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engel (Ref. 5.1)</td>
<td>50</td>
<td>$\phi$</td>
<td>350</td>
<td>400</td>
</tr>
<tr>
<td>Esch (Ref. 5.2)</td>
<td>120</td>
<td>$\phi$</td>
<td>397</td>
<td>517</td>
</tr>
<tr>
<td>Present Investigation</td>
<td>3</td>
<td>1</td>
<td>388</td>
<td>392</td>
</tr>
</tbody>
</table>

$\phi$ Did not consider

$Q^*$ watts/cm$^2$

heat transfer by diffusion
compared, it becomes evident that they are markedly different and that finite-rate chemistry effects are present throughout the flow-field.

(The complete set of dimensionless temperature, enthalpy, density, velocity and mass fraction profiles for the two non-equilibrium and the equilibrium runs are presented in Appendix C. Those profiles needed in the following discussion will be reproduced in this chapter.)

An examination of the chemical composition of equilibrium ablation products shows that as they leave the char surface and are subjected to rapidly increasing temperatures, the decomposition process begun in the char continues as the "large" molecules, \( \text{C}_3\text{H}, \text{C}_2\text{H}, \text{C}_4\text{H}, \text{HCN}, \text{C}_2\text{H}_2, \) and \( \text{H}_2 \) are broken down (for example see Fig. 5.1) into simpler species such as \( \text{C}_3, \text{C}_2, \text{CO}, \text{CN}, \text{N}_2, \) C and H (see Fig. 5.2). As the ablation products flow towards the stagnation point, this process continues as \( \text{C}_3, \text{C}_2, \text{CO}, \text{CN}, \) and \( \text{N}_2 \) are converted to \( \text{C}, \text{C}^+, \text{N}, \) and O (see Figs. 5.2 and 5.3).

Near the stagnation point, most of the carbon is ionized to \( \text{C}^+ \) and, due to diffusion of ablation products past the stagnation point, the concentration of \( \text{C}^+ \) persists for some distance past the stagnation point before decreasing to zero (see Figs. 5.3 and 5.4).

In the region from the char surface to the stagnation point the non-equilibrium results predict that the ablation products will decompose at a much slower rate, when compared to the rate predicted by the equilibrium results. The "large" molecules (\( \text{C}_3\text{H}, \text{C}_2\text{H}, \text{C}_4\text{H}, \text{HCN}, \text{C}_2\text{H}_2, \) and \( \text{H}_2 \)) and others (\( \text{C}_3, \text{CO}, \text{CN}, \) and \( \text{N}_2 \)) begin to break down into \( \text{C}, \text{C}^+, \text{C}_2, \text{N}, \text{N}^+, \text{O}^+, \) and H (see Figs. 5.1, -5.3). But the ablation products reach the stagnation point before this process is completed and the results are much lower concentrations of \( \text{C}, \text{C}^+, \text{N}, \text{O}, \) and H in
Figure 5.1 Mass Fraction Profiles for C₃H
Figure 5.2 Mass Fraction Profiles for C₃
Figure 5.3 Mass Fraction Profiles for C
Figure 5.4 Mass Fraction Profiles for $C_i^+$
this region (see Fig. 5.4).

In the shock layer region of the flow-field, equilibrium results predict that as the air components are cooled down a process of rapid de-ionization occurs with most of the $\text{N}^+$ and $\text{O}^+$ being converted to $\text{N}$ and $\text{O}$ (see Figs. 5.5 and 5.6). On the other hand, non-equilibrium results predict that the air components will flow from the shock to the stagnation point without undergoing any changes until very close to the stagnation point where their concentrations begin to decrease and fall rapidly past the stagnation point. As a result of these "frozen" concentrations, the region between the shock and the stagnation point has much lower concentrations of $\text{N}$ and $\text{O}$ (and much higher concentrations of $\text{N}^+$ and $\text{O}^+$) than those predicted by the equilibrium analysis (see Figs. 5.5 and 5.6).

Therefore, the non-equilibrium analysis predicts much lower concentrations of $\text{C}$, $\text{CN}$, $\text{C}^+$, $\text{N}_2$, $\text{N}$, $\text{O}$, and $\text{H}$ and much higher concentrations of $\text{C}_2$, $\text{CO}$, $\text{C}_3\text{H}$, $\text{C}_2\text{H}$, $\text{C}_4\text{H}$, $\text{HCN}$, $\text{C}_2\text{H}_2$, $\text{N}^+$, $\text{O}^+$, $\text{H}_2$, and $\text{e}^-$ than the equilibrium analysis. Since $\text{C}$, $\text{N}$, $\text{O}$, and $\text{H}$ line and continuum mechanisms are the major contributors to radiative energy transport in the shock layer (Ref. 5.4), under non-equilibrium chemistry conditions the resulting radiative heat transfer to the body is significantly lower than the one predicted by chemical equilibrium analyses.

**DIFFICULTIES ASSOCIATED WITH THE SOLUTION**

This research demonstrates that the speed of obtaining a solution, if one can be obtained, depends on a large number of factors including: the formulation of the model, how realistic the values used for properties are, the numerical techniques used, and how such techniques are implemented.
Figure 5.5 Mass Fraction Profiles for $N^+$

- Equilibrium (SLAC)
- Non-Equilibrium (Balhoff)
- Non-Equilibrium (SLAC)

The stagnation point is indicated on the graph.
Figure 5.6 Mass Fraction Profiles for N
The attempts at using the energy equation in terms of temperature failed because the temperature profile is very sensitive to the values of the other dependent variables and the energy equation in this form is apparently more strongly coupled to the species equations. The enthalpy formulation, on the other hand, permits uncoupling of the equations and makes it possible to obtain a converged solution.

However, although a solution was determined using the energy equation in terms of enthalpy, obtaining such a solution was extremely difficult. Much of this difficulty arose because of the use of unrealistically high reaction rates. The non-equilibrium solution using the original chemical kinetics model took about 18 hours of time in an IBM 360/65 computer. The solution using the modified kinetics model took about 45 minutes in the same computer. This means that the unrealistic rates increased the difficulty in obtaining a solution.

As was discussed in Chapter 4, a number of numerical techniques have been demonstrated to be inappropriate for solving chemical kinetics problems. However, even those techniques which may be valid will not work unless they are implemented properly. For example, the scheme used to uncouple and iterate on the equations will, in many cases, make the difference between success and failure. Also, the weighting factors used to obtain new guesses from the old and new solutions (the $\lambda$'s in Figs. 4.1 - 4.4) determine if the solution will converge. Unfortunately, there is no straightforward procedure for determining how to implement a technique properly; a great deal of experimentation is required before success is attained.
REFERENCES

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5.2 Esch, Donald D., Stagnation Region Heating of a Phenolic-Nylon Ablator During Return from Planetary Missions, Ph.D. Dissertation Louisiana State University, Baton Rouge, Louisiana (1971).

5.3 Balhoff, John F., Research Associate, Chemical Engineering Department, Louisiana State University, Private Communication.

5.4 Engel, op. cit., Vol. I, p. 126
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

From the results obtained in the present investigation the following conclusions can be derived:

A finite-rate stagnation-line shock layer solution which contains a reasonable kinetics model to describe atmospheric entries protected by phenolic-nylon ablators was developed.

The model was used to determine the non-equilibrium shock layer structure and body heating rates under flight conditions typical of return from planetary missions. Although only one set of conditions was considered, it is believed that the method of solution is adequate for a range of conditions similar to the ones considered.

2. Finite-rate chemistry effects are significant for the flight conditions considered.

The results obtained show that as the ablation products enter the shock layer they react much slower than under equilibrium conditions. The air components entering through the shock are not de-ionized, as the equilibrium analysis predicts, but remain "frozen" throughout most of the shock region. The validity of these results are, of course, dependent upon the accuracy of the chemical kinetics model used. The degree of confidence in the results is high because: the kinetics model used is
the most complete that has been used in this type of application, the re-
action rates used were the best rates available, and for both sets of re-
action rates (the original and the modified) the same finite-rate chem-
istry effects were present.

3. For the flight conditions studied the total heating rate
to the body is significantly lower under non-equilibrium
than under equilibrium chemistry conditions.

The predicted non-equilibrium heating rate is approximately one
third as large as the predicted equilibrium heating rate. This results
from the fact that the non-equilibrium radiative heating rate is approxi-
mately one third as large as the equilibrium radiative heating, and in
both instances, most of the total heating results from radiation. The
significantly lower radiative heating rate is a direct result of finite
rate chemistry effects which result in much lower concentrations of C,
N, O, and H, the species responsible for most of the line and continuum
radiative transfer.

RECOMMENDATIONS

Considering the conclusions presented above, it is recommended that:

1. The mathematical model for the stagnation-line analysis
of an entry vehicle presented herein should be studied
further to determine if its computational speed can be
increased.

The present version of SLAC should be developed from the research
tool it is today until it becomes an effective engineering tool. The
principal obstacle that needs to be overcome is the amount of computer
time required to obtain a solution. The computational speed is a func-
tion of: the model formulation, how realistic the properties used are,
the schemes for uncoupling and iterating on the equations, and the numerical techniques used. Much improvement in computational speed was obtained by considering different variations on all these factors. It is believed that the computational speed of the present solution could be increased by at least a factor of 2 by further consideration of uncoupling and iterating schemes.

2. Studies of finite-rate chemistry effects be carried out under flight conditions different from those considered in the present work.

The objectives of the proposed studies should be to determine: a) the range of flight conditions over which solutions may be obtained using the implemented model; and b) the range of conditions over which finite-rate chemistry effects are significant and how they affect the heating rates to the body.

3. Research be carried out on the effect of assuming more realistic shock and wall boundary conditions.

This investigation should consider using non-equilibrium compositions of air at the shock as boundary conditions and using boundary conditions of the third kind at the wall. The use of non-equilibrium compositions of air will result in increased concentrations of N and O and less N⁺ and O⁺ when compared to the equilibrium boundary conditions. This might result in increased radiative heating rates since N and O are optically more active than N⁺ and O⁺. By perturbing the shock boundary conditions used in SLAC an estimate of the importance of this effect could be developed. In the present investigation the mass and energy boundary conditions used at the wall were of the first kind, however the mass and energy surface balances yield conditions of the third kind.
A study should be carried out to determine if using the more complete conditions has any significant effect on the heating rate.

4. Coupled solutions for both non-equilibrium ablation products and shock layers should be determined.

A complete solution to the quasi-steady entry problem requires that the ablator response be coupled to the existing flight conditions through the shock layer. This can be accomplished by performing multiple calculations of ablation and shock layer behaviour and matching conditions at the interface between the ablator surface and the flow field. At present, ablator-shock layer response under chemical equilibrium conditions has been studied, however, additional studies should be carried out coupling the finite-rate solutions determined from SLAC to those obtained from a non-equilibrium ablator-response model.
APPENDIX A

USER'S MANUAL FOR SLAC

INTRODUCTION

This appendix will serve as a user's manual for the SLAC (Stagnation Line Analysis with Chemistry) program. The program implements a model designed to predict the stagnation line viscous, reactive, and radiative coupled shock layer structure, and the resulting heating rates produced by a blunt body during super orbital entry into planetary atmospheres. The problem was formulated in Chapter 1, and the equations describing the flow-field (the stagnation line boundary layer equations (See Table 2.7), and the wall and shock boundary conditions (See Table 2.8), were derived in Chapter 2. The thermodynamic, transport, radiative, and chemical kinetic properties are described in Chapter 3. The program can also be used to compute flows in chemical equilibrium, and for this purpose it utilizes a free energy minimization routine developed by Del Valle and Pike (Ref. A.1). The numerical procedures used to solve the model are described in Chapter 4.

The SLAC program results from extensions performed on a program (VISRAD) primarily developed by Engel (Ref. A.2), and in a program (SLAB) developed by Esch (Ref. A.3) from VISRAD. These programs result from the efforts of many individuals over a considerable period of time. SLAC was designed to be used for thermal environment prediction studies. It
represents a significant tool for studying a variety of atmospheric en­
try heating problems. The program, written in FORTRAN IV, is capable of performing the following types of analyses:

- Stagnation line solutions
- Coupled diffusive, convective and radiative flux calculations
- Emission, and line and continuum radiation calculations
- Binary diffusion calculations
- Finite-rate or equilibrium chemistry calculations

PROGRAM PROCEDURES

The SLAC computer program was developed following a philosophy of minimizing user's effort and maximizing program flexibility and adaptability. Accordingly, the basic program logic as shown in Figure A.1 is quite simple. However these basic subprograms are supported by 22 sub­routines and 7 function subprograms. Each of these modules performs computational functions which are of a basic nature (e.g., computation of thermodynamic properties), and allows for modification, substitution, addition or deletion of existing modules with minimum effort.

In order to minimize input requirements, three techniques were used. The first consists of internal initialization of values for temperature, density, viscosity, and stand-off distance which are necessary to start the solution procedure. If better guesses are available they may be input as discussed in the next section. The second technique involves internal specification in BLOCK DATA of problem-defining parameters such as the elemental composition at the surface and thermodynamic curve-fit constants which are changed quite infrequently. The third technique consists of internally selecting program options if an option variable is left blank on an input card. In this procedure the most commonly used options are performed when a blank is input.
(INPUT)*
Read All Input

First Iteration?
Yes

(INIT)
Compute Necessary Initial Quantities

(MOMIM)
Solve Equations of Momentum and Global Continuity

(COUPLE)
Solve Equations of Energy and Species Continuity

(OUTPUT)
Print Intermediate Results

(PONCH)
Punch Intermediate Results

Converged Solution?

Yes

(OUTPUT)
Print Results

* Names in parenthesis refer to program subroutines
The start up of the SLAC program can be achieved in a number of ways. As stated previously, internal guesses are available to begin the iteration procedure. Two types of temperature profiles are available. One for no mass injection and the other for mass injection. These profiles are usually quite satisfactory as initial guesses if an emission radiation coupled problem is to be run. However, if a line and continuum radiation coupled problem which includes mass injection, and finite-rate chemistry is to be run the internal guess may not be accurate enough. Consequently, it might be necessary to input a better temperature profile guess.

**INPUT GUIDE**

All inputs to the SLAC computer program are read from cards supplied by the user; no tapes are required. The basic inputs consist of parameters defining flight conditions (free-stream velocity and density), blunt body radius, wall temperature and mass injection rate. Additional input parameters are required to determine which program options are desired, and to provide the necessary guesses of dependent variables. After each overall iteration, the program outputs a deck of cards containing the values of the dependent variables and other pertinent parameters in such a manner that a given case run may be interrupted and continued at a later time by using the produced deck of punched cards to restart the run. Multiple case runs, and hence entire trajectories, can be processed by placing the input data for each new case behind the data for the previous one.

Table A.1 presents the card input formats for SLAC and Table A.2 provides a corresponding definition of variables.

In single case runs Card 10 must be followed by a card with the characters END punched in columns 1, 2 and 3 to indicate the run has ended. In multiple case runs the END card should be placed after Card
<table>
<thead>
<tr>
<th>Card</th>
<th>Variables</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>TITLE, IEM</td>
<td>18A4, I8</td>
</tr>
<tr>
<td>2</td>
<td>KEEP, NETA, IRAD, ITYPE, MAXM, MAXE, MAXD, LT, IPHI, FPRCT, TPRCT, IDEBUG</td>
<td>915, 2E12.0, 2X, I1</td>
</tr>
<tr>
<td>3</td>
<td>UNIF, RINF, R, TWK, HTOTAL, RVW</td>
<td>6E12.0</td>
</tr>
<tr>
<td>4</td>
<td>DELTA, DTIL, RZB, RE, PDTIL</td>
<td>5E12.0</td>
</tr>
<tr>
<td>5</td>
<td>T(I)</td>
<td>6E12.0</td>
</tr>
<tr>
<td>6A</td>
<td>RH(I)</td>
<td>6E12.0</td>
</tr>
<tr>
<td>6B</td>
<td>RM(I)</td>
<td>6E12.0</td>
</tr>
<tr>
<td>7</td>
<td>DEPS</td>
<td>E12.0</td>
</tr>
<tr>
<td>8</td>
<td>ETA(I)</td>
<td>6E12.0</td>
</tr>
<tr>
<td>9</td>
<td>NDEBUG, TOL, IAB</td>
<td>I5, 5X E10.4, I5</td>
</tr>
<tr>
<td>10</td>
<td>CWALL(J)</td>
<td>5E15.8</td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>1</td>
<td>TITLE</td>
<td>Title for identification of the problem</td>
</tr>
<tr>
<td></td>
<td>IEM</td>
<td>Number of overall iterations performed. IEM = 0 for case run initiation, IEM&gt;0 for restarts</td>
</tr>
<tr>
<td>2</td>
<td>KEEP</td>
<td>Indicator to determine if the temperature profile from the previous case is to be kept as a guess for the current case.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KEEP = 0 Temperature not kept</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KEEP = 1 Temperature kept</td>
</tr>
<tr>
<td></td>
<td>NETA</td>
<td>The number of points to be used in the shock layer profile. If NETA = 0, a set of 51 equally spaced points will be used. If NETA&gt;0 card 8 must be read.</td>
</tr>
<tr>
<td></td>
<td>IRAD</td>
<td>A variable used to specify the type of solution.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IRAD = 1 Convective solution only</td>
</tr>
<tr>
<td></td>
<td></td>
<td>= 2 Uncoupled radiation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>= 3 Coupled radiation solution</td>
</tr>
<tr>
<td></td>
<td>ITYPE</td>
<td>A variable used to specify the type of radiation model to be used.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ITYPE = 0 Line and continuum radiation model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>= 1 Emission radiation model</td>
</tr>
<tr>
<td></td>
<td>MAXM</td>
<td>Maximum number of iterations allowed in the internal momentum loop. If MAXM = 0, it is internally set = 15.</td>
</tr>
<tr>
<td></td>
<td>MAXE</td>
<td>Maximum number of iterations allowed in the energy-species continuity equation and in the overall momentum-energy-species loop. If MAXE = 0, it is internally set = 15.</td>
</tr>
<tr>
<td></td>
<td>MAXD</td>
<td>Maximum number of iterations allowed in the external momentum loop. If MAXD = 0, it is internally set = 15.</td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>LT</td>
<td>Indicator to determine if a temperature guess and if ( \rho ) and ( \rho v ) guesses are to be read in.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LT = 0 Cards 5 and 6 are not read.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LT = 1 Card 5 but not card 6 is read.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LT = 2 Cards 5 and 6 are read.</td>
<td></td>
</tr>
<tr>
<td>IPHI</td>
<td>Indicator to determine if the shock curvature is to be input.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>IPHT = 0 ( dc/d\epsilon ) = 0 is internally set.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>IPHT = 1 Card 7 is required for input.</td>
<td></td>
</tr>
<tr>
<td>FPRCT</td>
<td>Convergence tolerance for each point the ( f' ) profile. If FPRCT = 0.0 it is internally set = .005.</td>
<td></td>
</tr>
<tr>
<td>TPRCT</td>
<td>Convergence tolerance for each point in the ( T ) profile. If TPRCT = 0.0, it is internally set = .005.</td>
<td></td>
</tr>
<tr>
<td>IDEBUG</td>
<td>A switch to allow intermediate printout to be obtained at each iteration</td>
<td></td>
</tr>
<tr>
<td></td>
<td>IDEBUG = 0 No print.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>IDEBUG = 1 Print is given</td>
<td></td>
</tr>
<tr>
<td>3 UNIF</td>
<td>The free-stream flight velocity ( (U_\infty) ) in feet/sec.</td>
<td></td>
</tr>
<tr>
<td>RINF</td>
<td>The free-stream density ( (\rho_\infty) ) in slugs/ft(^3).</td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>Principal body radius in feet.</td>
<td></td>
</tr>
<tr>
<td>TWK</td>
<td>Wall Temperature in degrees Kelvin.</td>
<td></td>
</tr>
<tr>
<td>HTOTAL</td>
<td>Total free-stream enthalpy in ft(^2)/sec(^2).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>If HTOTAL = 0.0, it is set to ( U_\infty^2/2 ). (Free-stream static enthalpy is assumed negligible).</td>
<td></td>
</tr>
<tr>
<td>RVW</td>
<td>Mass injection rate ( (\rho v)<em>{w}/(\rho U</em>\infty) ).</td>
<td></td>
</tr>
<tr>
<td>4 DELTA</td>
<td>An initial guess for the shock standoff distance ( S/R ). If DELTA = 0.0, a guess is supplied by program.</td>
<td></td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>DTIL</td>
<td>A guess for the transformed standoff distance $\delta/R$. The program will also supply this value if DTIL 0.0</td>
<td></td>
</tr>
<tr>
<td>RZB</td>
<td>The density ratio across the shock $\bar{\rho}=\rho_\infty/\rho_\delta$. If RZB is input as 0.0, the code will determine a value.</td>
<td></td>
</tr>
<tr>
<td>RE</td>
<td>The Reynolds number for the problem, $Re_s = U_\infty \rho_\delta/\mu_\delta$. This quantity is determined by the program if RE is input as 0.0.</td>
<td></td>
</tr>
<tr>
<td>PDTIL</td>
<td>Convergence tolerance placed on $\delta$ for total solution convergence. If PDTIL = 0.0, it is internally set = 0.01.</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>T(I), I = 1, NETA</td>
<td>An initial guess for the dimensionless shock layer temperature profile ($T/T_\delta$). This card is required only if LT&gt;0.</td>
</tr>
<tr>
<td>6A</td>
<td>RH(1), I=1, NETA</td>
<td>An initial guess for the dimensionless shock layer density profile ($\rho/\rho_\delta$). This card is required only if LT = 2.</td>
</tr>
<tr>
<td>6B</td>
<td>RM(I), I=1, NETA</td>
<td>An initial guess for the dimensionless shock layer $\rho v$ profile ($\rho v/\rho_\delta v_\delta$). This card is required only if LT = 2.</td>
</tr>
<tr>
<td>7</td>
<td>DEFS</td>
<td>The stagnation line shock curvature ($d\delta/dx$). If IPHI = 0, then $d\delta/dx = -0.0$ is internally set. If IPHI = 1, Card 7 is read and $d\delta/dx$ is supplied by the user.</td>
</tr>
<tr>
<td>8</td>
<td>ETA(I), I=1, NETA</td>
<td>The grid shock layer points at which the solution profiles are to be computed. If NETA = 0, $\Delta \eta$ is set to 0.02 and ETA (I) is computed by the program. (ETA(1)=0.0+ wall, ETA (NETA)=1.0+ shock).</td>
</tr>
<tr>
<td>9</td>
<td>NDEBUG</td>
<td>Debug option to output thermodynamic curve-fit equations and intermediate results from NDEBUG = 0 No output. NDEBUG = 1 Output given.</td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>-----------------</td>
<td>-------------</td>
</tr>
<tr>
<td></td>
<td>TOL</td>
<td>Convergence criteria for CHEMQ. If TOL is input as 0.0, the code will set it to 0.001.</td>
</tr>
<tr>
<td></td>
<td>IAB</td>
<td>A variable used to specify the type of chemistry model to be used.</td>
</tr>
<tr>
<td></td>
<td>CWALL(J),</td>
<td>Wall mass fractions.</td>
</tr>
<tr>
<td></td>
<td>J=1,NSP</td>
<td>NSP = 20</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>J = 1→O₂, 6→N⁺, 11→CO, 16→C₃H</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2→N₂, 7→E⁻, 12→C₃, 17→C₄H</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3→O, 8→C, 13→CN, 18→HCN</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4→N, 9→H, 14→C₂H, 19→C₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5→O⁺, 10→H₂, 15→C₂H₂, 20→C⁺</td>
</tr>
</tbody>
</table>
Some caution should be exercised when preparing an input for this program. The program considers 5 elements, including electrons, and twenty species listed under CWALL (J). The set of species was selected for an air atmosphere and an phenolic-nylon ablator. If another ablator is selected for study and this set of species is appropriate, no alteration of the program is required. All that is required is a card input of wall mass fractions of the ablator selected on Card 10. If extensive study of a different ablator using this program is anticipated, the user may find it convenient to change the wall composition stated in BLOCK DATA under CWALL rather than reading in the data for each run.

If required, a change to another set of species can be made with comparatively little difficulty. Thermodynamic and transport properties may be altered by changing the curve-fit constants in BLOCK DATA. The thermodynamic curve-fit equations were listed in Table 3.1 and the correspondence between the coefficients in the table and those in the program is

For

\[
\begin{align*}
1000 < T \leq 6000 & \\
A_1 & = \quad A_1 & = \quad A_{11} \\
A_2 & = \quad B_{11} \\
A_3 & = \quad C_{11} \\
A_4 & = \quad D_{11} \\
A_5 & = \quad E_{11} \\
A_6 & = \quad F_{11} \\
A_7 & = \quad G_{11}
\end{align*}
\]

where the coefficients are dimensioned to include a value for each species.
The species ordering is given in the SP array with corresponding ordering in SMW (i.e. species molecular weight) array in BLOCK DATA. The transport properties curve-fit equations are listed in Tables 3.3 (viscosity) and 3.4 (thermal conductivity) and the correspondence between the coefficients in those tables and those in the program is:

Viscosity:

<table>
<thead>
<tr>
<th>Table 3.3</th>
<th>SLAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>a = V1</td>
<td></td>
</tr>
<tr>
<td>b = V2</td>
<td></td>
</tr>
<tr>
<td>c = V3</td>
<td></td>
</tr>
</tbody>
</table>

Thermal Conductivity

<table>
<thead>
<tr>
<th>Table 3.4</th>
<th>SLAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>a = K1</td>
<td></td>
</tr>
<tr>
<td>b = K2</td>
<td></td>
</tr>
</tbody>
</table>

If new species and reactions are to be included in the finite-rate calculations, then subroutine FG2 must be modified accordingly. Finally, a study should be made to determine if radiatively important species are to be included.

OUTPUT DESCRIPTION

This section presents a description of the program output and definitions of the output symbols. The program produces both printed output and punched card output. The printed output provides a human-readable record of input parameters, intermediate results and the final solution. The punched card output provides a machine-readable medium for restarting runs.

Printed Output

The first page of output is a print of the input data. This is provided for a check of the input and an identification of the problem.
All quantities on this page are defined in the Input Guide section.

Most of the second page also contains problem specification data which is self explanatory. Following the guessed nondimensional stand-off distance (DELTA) and transformed stand-off distance (DELTA) and transformed stand-off distance (DTIL), a listing of the dimensional stand-off distance computed at each iteration is given if the line-continuum radiation model is used.

Species number densities for those species used in the radiation calculation during the final iteration are printed on the third page.

The fourth page provides an output of radiative fluxes computed during the final iteration. The continuum contribution and line contribution to the spectral flux is printed for three ETA points (ETA = 0.0 = wall, ETA = stagnation point, ETA = 1.0 = shock) as a function of frequency intervals and frequency centers respectively. The columns of fluxes in watts/cm² denoted by Q PLUS and Q MINUS designates fluxes toward the surface and away from the surface respectively.

From the fifth until the thirtieth page, results of the overall iteration, either final or intermediate, are presented. The fifth page begins with one of the following messages: (1) "INTERMEDIATE PRINT AT ITERATION NO. a MCONV = b ECONV = c DCONV = d" where a is the overall iteration number, and b, c, and d are either T (true) or F (false) depending upon if the momentum - global continuity equation, energy-species continuity equations, and the shock stand-off distance have converged, respectively. If this message is printed at least one of b, c, or d must be F. (2) "SOLUTION CONVERGED IN e ITERATIONS", where e is the number of overall iterations it took to converge. Following either one of these two messages is a printout of the shock stand-off distance parameters DELTA, DTIL; the convective (QC), radiative (QR), diffusive
(QD) and total heating rate with the respective units printed. To the
left of the heating rate data the density ratio across the shock (RB)
and the mass injection rate (RWV) are stated. Following the heating
rate data is a print of some of the solution profiles as a function of
the shock layer coordinates ETA and (Y/D). The solution profiles printed
are:

F' = velocity function
RV = ρU/ρ∞, U (nondimensional mass flux per unit area)
T/TD = T/T∞ (nondimensional temperature)
E = 1E (radiative flux divergence)
V = V/U∞ (nondimensional normal velocity)
V(FT/SEC) = dimensional normal velocity
G = nondimensional total enthalpy
H(STATIC) = nondimensional static enthalpy

These profiles appear in part of page 5 and in page 6.

The shock layer thermodynamic and transport properties as a func­tion of ETA and Y/D are printed in the following pages. The profiles
printed are:

P(ATM) = pressure in atmospheres
T(⁰KEL.) = temperature in degrees Kelvin
RHO (SLUGS/FT3) = density in slugs/cubic feet
M (LBM/FT-SEC) = viscosity in lbm/(ft-sec)
RM (LBF2-SEC3/FT6) = product of density and viscosity in

1lb² - sec³/ft⁶

K(BTU/FT-SEC-R) = thermal conductivity in Btu/(ft-sec-⁰R)

The next four pages present the profiles of the mass fractions of
O₂, N₂, O, N, O⁺, N⁺, e⁻, C, H, H₂, CO, C₃, CN, C₂H, and C₂H₂ as a func­tion of ETA. Page 13 contains the profiles of mixture specific heat at
constant pressure (CP), mass fractions for $C_3H$, $C_4H$, HCN and $C^+$, and the mixture molecular weight (AMW) as a function of ETA.

The above description is for a standard output. However, if the intermediate print option is used (i.e. IDEBUG > 0) or if the thermodynamic fits and intermediate results from the chemical equilibrium calculation are desired (i.e. NDEBUG = 1), additional information is printed.

If message number (2) is printed, the run has ended and the program proceeds to the next case or stops if there are no additional cases to be run. If message number (1) is printed, the solution has not converged and additional iterations must be carried out.

**Punched Card Output**

After each overall iteration the program outputs a deck of cards containing all relevant data on flight conditions, body characteristics, and shock layer structure. These data are punched by a subroutine named PUNCH in such a manner that the cards may be used to restart a run at a later time. For example, if the program is allowed to run for 3 hours, during that time the program might perform 4 overall iterations and it would output 4 decks of punched cards, one for each overall iteration. If the solution has not converged after the 3 hours have run out, the fourth deck of punched cards may be used to restart the run at a later time.

**REFERENCES**


C **** START OVERALL ITERATION ****
C
1000 CONTINUE
   IEM = IEM+1
C
   ** SOLVE MOMENTUM EQUATION **
   CALL MOMTM
C
   ** SOLVE ENERGY AND SPECIES EQUATIONS **
   CALL COUPLE
C
   ** INTERMEDIATE PRINTOUT **
   CALL OUTPUT (2)
   CALL PONCH
C
   ** CHECK SIMULTANEOUS MOMENTUM AND ENERGY CONVERGENCE **
   IF(IEM*GT*MAXD) GO TO 3000
   IF(*NOT*MCONV) GO TO 1000
   IF(*NOT*ECONV) GO TO 1000
   IF(*NOT*DCONV) GO TO 1000
   ** PRINT ALL OUTPUT **
   CALL OUTPUT (1)
C
   ** CONVERGED, GO BACK TO RUN ANOTHER CASE **
C
GO TO 1
C
3000 CONTINUE
C
** MOMENTUM AND ENERGY DID NOT CONVERGE SIMULTANEOUSLY **
C
CALL OUTPUT (3)
GO TO 1
END
SUBROUTINE INPUT
** ROUTINE TO READ AND PRINT ALL INPUT DATA **

COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
COMMON/CONV/ADAMP
COMMON /DEL/ DELTA,DTLS
COMMON /FISTRM/ U INF, RINF, UINF2, R, RE, LXI, ITM, IEM, NETA
COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,DEBUG,MCNV,ECONV,DCONV,LT,IA
COMMON /NON/MDZ,AMDZ,AKNF,HNF,CPNF
COMMON/PROP1/PI(60),RHO(60), T(60),AMW(60),C (20,60),CC(5,60)
COMMON/PROP2/ MU(60),RM(60), AK(60)
COMMON/PROP3/CPS(20,60),HS(20,60),CP (60),HM(60)
COMMON /RFLUX/ E(60),IRAD,ITYPE
COMMON /VEL/ F(60),FC(60),Z(60),V(60)
COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
COMMON/WALL/RW,PRW,TRW,FLUX(20),CWALL(20),ECWALL(5)
COMMON /YL/ETA(60),YCNO(60)
COMMON/TIT/TITLE(18)
COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20)
COMMON/EQ2/AA(20,5),ICODE(20)
COMMON/EQ3/IA(20,5)
COMMON/ID/SP(20),EL(5)
COMMON/WT/SWM(20),AWT(5)
COMMON/NUMBER/ASP,NNS,NE,NC
COMMON/SP1/SS,TOL,NDBGU

REAL MU,MUDZ
LOGICAL MCONVECONV,DCONV
DATA END */END */
** INPUT FORMATS **

100 FORMAT (18A4,1I8)
101 FORMAT (9I5,2E12.0,2X,I1)
102 FORMAT ( 6E12.0 )
107 FORMAT(I5, 5X,E10.4,I5)
108 FORMAT(5E15.9)

** OUTPUT FORMATS **

200 FORMAT ( 1H1 , 18A4,18 /// )
201 FORMAT ( 12H0 INPUT DATA /// )
202 FORMAT ( 9H0KEEP = I5
1 / 9H  NETA = I5
2 / 9H  MAXM = I5
3 / 9H  MAXE = I5
4 / 9H  MAXD = I5
5 / 9H  FPRCT = 1PE15.6
6 / 9H  TPRCT = E15.6
7 / 9H  LT = I5
8 / 9H  IDEBUG = I5
9 / 9H  IPHI = I5 )
203 FORMAT(1X/*  ** FINITE-RATE CHEMISTRY  **/ )
204 FORMAT ( 9H0UNF = 1PE15.6
1 / 9H  RINF = E15.6
2 / 9H  R = E15.6
3 / 9H  TW = E15.6
4 / 9H  HTOTAL = E15.6
5 / 9H  RVW = E15.6
6 / 9H  PDTIL = E15.6 ///
205 FORMAT ( 9H0DBG = I5
1 / 9H  TOL = F5.3/// )

206' FORMAT ( 20H0INITIAL- T PROFILE / ( 1H , 12F10.5 ) )
207 FORMAT ( 20H INITIAL RHO PROFILE/ ( I H , 12F10.5 ) ) INPU 710
208 FORMAT ( 20H0 INITIAL RM PROFILE/ ( I H , 12F10.5 ) ) INPU 720
209 FORMAT ( 20H0 ETA ) INPU 730
210 FORMAT (32H CONVETIVE CALCULATION ONLY * ) INPU 740
211 FORMAT (36H UNCOUPLED RADIATION CALCULATION * ) INPU 750
212 FORMAT (34H COUPLED RADIATION CALCULATION * ) INPU 760
213 FORMAT (36H CONTINUUM AND LINE CALCULATION * ) INPU 770
214 FORMAT (19H EMISSION MODEL * ) INPU 780
215 FORMAT(1X/ ** EQUILIBRIUM CHEMISTRY **/ ) INPU 790
216 FORMAT (16H SPECIES INPUTS)
   1 /16H NO. ELEMENTS = 15
   2 /25X5(I5,2X,A4) ) INPU 800
218 FORMAT (16H NO. SPECIES = I5)
220 FORMAT (25X5(I5,2X,A4)) INPU 810
222 FORMAT (16H NO. SOLIDS = I5)
C
C CARD 1 ------------------------ INPU 820
C RFAD (5,100) TITLE,IEM
   IF ( TITLE ( 1 ) *EQ* END ) STOP
   IF(IEM)6999,5999,6999
   5999 CONTINUE
C
C **** START FROM SCRATCH ****
C
C ** INPUT OPTION PARAMETERS **
C
C ** IRAD = 1 NO RADIATION CALCULATED **
C ** IRAD = 2 UNCOUPLED SOLUTION **
C ** IRAD = 3 COUPLED SOLUTION **
C ** ITYPE=0 SPECTRAL MODEL WITH LINES
C ** ITYPE=1 EMISSION MODEL
C
C KETA = NETA
C CARD 2 ------------------------ INPU 840
C
C
READ (5,101) KEEP, NETA, IRAD, ITYPE, MAXM, MAXE, MAXD, LT, IPHI, FPRCT, TPRCT, IDEBUG

META = NETA
IF(KETA EQ 0) KEEP = 0
IF(KEEP GT 0) NETA = KETA

HDAMP = 0.6
TDAMP = 0.06
DDAMP = 0.5
IF(MAXM EQ 0) MAXM = 15
IF(MAXE EQ 0) MAXE = 5
IF(MAXD EQ 0) MAXD = 15
IF(FPRCT EQ 0) FPRCT = 0.005
IF(TPRCT EQ 0) TPRCT = 0.005
IF(IRAD EQ 0) IRAD = 1

C ** FREE-STREAM FLIGHT CONDITIONS **
C CARD 3 -----------------------------------------------
READ(5,102) UINF, R INF, R, TWK, HTOTAL, RVW
UINF2 = UINF**2
IF(KEEP GT 0) TWOLD = T(1)
T(1) = TWK

C IF(HTOTAL EQ 0) HTOTAL = UINF2 / 2.0

C ** INITIAL SHOCK QUANTITY ESTIMATES **
C CARD 4 -----------------------------------------------
READ(5,102) DELTA, DTIL, RZB, RE, PDTIL
IF(PDTIL EQ 0) PDTIL = 0.01

C ** INPUT INITIAL TEMPERATURE PROFILE **
C CARD 5 -----------------------------------------------
IF(LT EQ 0) GO TO 2800
READ ( 5,102 ) ( T ( I ), I = 1, NETA )
2800 CONTINUE

** INPUT RHO AND (RHO)(MU) PROFILES **
C CARD 6

IF(LT.LT.2) GO TO 2900
READ(5,102) (RHO(1), I = 1, NETA)
READ(5,102) (RM (I), I = 1, NETA)
2900 CONTINUE

** SHOCK SHAPE (DEPS/DXI) **
C

IF (IPHI .NE. 0) GO TO 2550
DEPS = 0.0
GO TO 2570
2550 CONTINUE

** FIXED GRID SIZE CN ETA **
C

DETA = 0.02
ETA ( 1 ) = 0.0
DO 500 I = 2, NETA
ETA ( I ) = ETA ( I-1 ) + DETA
500 CONTINUE
GO TO 1500

1000 CONTINUE
C ** INPUT ETA POINTS **
C CARD 8
READ ( 5,102 ) ( ETA ( I ) , I = 1 , NETA )
C
1500 CONTINUE
C
C------READ SPECIES PARAMETER CARDS......
C CARD 9
READ 107, NDBG,TOL,IAB
C
IF(TOL.LE.0.0) TOL = .001
C NDBG=OPTIONAL OUTPUT VARIABLE
C NC = NUMBER OF GASEOUS COMPONENTS
C
CARD 10
READ 108,(C WALL(I),I=1,NSP)
GO TO 7999
6999 CONTINUE
C
**** RE-START ****
C
READ(S,1801) FPRCT,TRRCT,DDAMP,TDAMP,PTIL,HDAMP
READ(S,1801) DELTA,DTIL,DTILS
READ(S,1802) U INF,RINF,UNF2,R,RE,ITM,LEM,NETA
READ(S,1803) KEP,MAXM,MAX0,IDEBUG,MCONV.ECONV,DCONV,LT,IAB
READ(S,1801)RDZ,MUDZ,RMDZ,AKNF,HNF,CFNF
READ(S,1804) NSP,NSM,NE,NC
READ(S,1801) (PI(J),RHO(J),T(J),J=1,NETA)
READ(S,1901)(AMW(J),J=1,NETA)
READ(S,1801) ((C(I,J),J=1,NETA),I=1,NSP)
READ(S,1801) ((H M(J),J=1,NETA),I=1,NSP)
READ(S,1801) (E(J),J=1,NETA)
READ(S,1804) IRAD,IYPE
READ(S,1801)DUD,DPHI,TD,RZB,PD,HD,HTOTAL
READ(S,1801)(F(J),FC(J),Z(J),V(J),J=1,NETA)
READ(5,1801)RVW,PRW,TWOLD
READ(5,1801)(CWALL(I),I=1,NSP)
READ(5,1801)(ECWALL(K),K=1,NE)
READ(5,1801)(ETA(J),YGET(J),J=1,NETA)
READ(5,715)NBUG,IA8,TOL
READ(5,1801)(CC(J),J=1,NETA),K=1,NE)
1801 FORMAT(6E13.5)
1802 FORMAT(5E12.5,3I3)
1803 FORMAT(5I5,3F3.2)
1804 FORMAT(4F4.4)
715 FORMAT(2I5,E15.6)
C 7999 CONTINUE
C **** PRINT DATA ****
C WRITE ( 6,200 ) TITLE,IEV
WRITE ( 6,201 )
WRITE ( 6,202 ) KEEP,NETA,MAMX,MAXE,MAXD,FPRCT,TPRCT,LT,IDEBUG
WRITE(6,204)UINF,INF,TWKH,TOTAL,RVW,PDTIL
IF (IRAD.EQ.1) WRITE (6,210)
IF (IRAD.EQ.2) WRITE (6,211)
IF (IRAD.EQ.3) WRITE (6,212)
IF(IRAD.EQ.1) GO TO 300
IF( ITYPE.EQ.0) WRITE(6,213)
IF(ITYPE.EQ.1) WRITE(6,214)
300 CONTINUE
WRITE ( 6,206 ) ( T ( I ) , I = 1 , NETA )
IF (IF=EO.EQ.0) T(1) = TWK
WRITE (6,207) (RHOD(I),I=1,NETA)
WRITE (6,208) (RM(I),I=1,NETA)
WRITE (6,209) (ETA(I),I=1,NETA)
WRITE(6,217) DEPS
217 FORMAT(9HODEPS/DX1/(IH *12F10.) 31H)
IF(IAB.EQ.0) WRITE (6,203)
IF(IAB.EQ.1) WRITE (6,215)
WRITE(6,205) NDBUG,TOL
WRITE(6,216) NE*(I*EL(I), I=1,NE)
WRITE(6,218) NSP
JJ = 1
KK = JJ + 4
30 WRITE(6,220) (ISP(I), I=JJ,KK)
IF(KK+5.GT.NSP) GO TO 35
JJ = JJ + 5
KK = KK + 4
GO TO 30
35 KD = NSP - KK
IF(KD.LE.0) GO TO 45
KK = KK + KD
JJ = JJ + 5
40 GO TO 30
45 CONTINUE
WRITE(6,222) NNS
PRINT 305
305 FORMAT(/, 'SPECIES', NAME, '9X', 'SMW', '2X', 'WALL MASS FRACTION*/)
DO 10 I=1,NSP
10 PRINT302,ISP(I),SMW(I),C*WALL(I)
302 FORMAT(1X,A4,9F13.3,E12.4)
IF(NDBUG.EQ.0)GOTO9999
PRINT309
309 FORMAT(/, 'SPECIES',35X, 'THERMO-CONSTANTS A-G',29X, 'RANGE*/)
DO 11 I=1,NSP
11 PRINT303,ISP(I),AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)
303 FORMAT(/,1X,A4,7E12.4, ' LOW RANGE*/)
304 FORMAT(5X,7E12.4, ' HIGH RANGE*/)
PRINT 307
307 FORMAT(/,25X, 'AA(I,J) MATRIX*/)
DO12J=1,NE
12 PRINT 306,(IA(I*J),I=1,NSP)
306 FORMAT(5X,20I5)
C
9999 CONTINUE
RETURN
END
SUBROUTINE INIT

** ROUTINE TO COMPUTE NECESSARY INITIAL QUANTITIES**

COMMON /CONV/ FPRCT, TPRCT, DDAMP, TDAMP, PDTIL
COMMON /DEL/ DFLTA, DTIL, DTILS
COMMON /EQ2/ AA(20+5), ICODE(20)
COMMON /EQ3/I A(20+5)
COMMON /FRSTRM/ U INF, R INF, U INF2, R, RE, LXI, ITM, IEM, NETA
COMMON /GUESS/ TGI(60), TGZ(60)
COMMON /MAIM/ KEEPMAX, MAXM, MAXO, IDEBUG, MCONV, ECONV, DCONV, LT, IAB
COMMON /NON/ RDZ, MUDZ, RMDZ, AKNF, HMF, CFNF
COMMON /PROP1/ PI(60), RHG(60), T(60), AMW(60), C(20,60), EC(5,60)
COMMON /PROP2/ MU(60), RM(60), AK(60)
COMMON /PROP3/ CPS(20,60), HS(20,60), CP(60), HM(60)
COMMON /VECTOR/ CA(60), CB(60), CC(60), B(60)
COMMON /VEL/ F(60), FC(60), Z(60), V(60)
COMMON /RFLUX/ E(60), IRAD, ITYPE
COMMON /RH/ DUD, DPHI, TD, RZB, PD, HD, HTOTAL
COMMON /SP2/ BR, S(20), CSHOCK(5)
COMMON /WALL/ TVW, PRW, TWOLD, FLUX(20), CWALL(20), ECWALL(5)
COMMON /WT/ SMW(20), AWT(5)
COMMON /YL/ ETA(60), YCND(60)
COMMON /DD/D(60)
COMMON /IT/ AC
REAL MU, MUDZ

LOGICAL MCONV, ECONV, DCONV

MCONV = .FALSE.
ECONV = .FALSE.
DCONV = .FALSE.
DO 900 I=1,60
DO 900 J=1,NSP
900 C(J,I) = 1.0E-20

C
C ** DETERMINE DENSITY RATIO, REYNOLDS NUMBER
C FROM INPUTS OR RANKINE HUGONIOT EQS. **
C
C GUESSED VALUES
TD = 12000 + .5E-5*(HTOTAL -5.5E+8)
RZB= 0.06

C
T(NETA) = 1.0
HNF = 2*778*28*32*172/UINF2

CONTINUE
PD = (1.0 -RZB)*RINF *UINF2/2116*
HD = HTOTAL/(778*28*32*172)
CPNF = 1.8*778*28*32*172*TD *2. /UINF2
AKNF = 1.8*778*28*TD /RZB/(R*RINF*UINF*UINF2)
P(NETA) = PD
CALL GAS(NETA)
RZBI=RINF/(RDZ*RHO(NETA) )
TEST =ABS((RZB-RZBI)/RZB)
IF(TEST LT 0.0005) GO TO 999
RZB=.5*(RZB+RZBI)
GO TO 998

CONTINUE
RE = RDZ*UINF*R*32*174 / MUDZ

C
C ** GUESS AT DELTA TO START **
C
IF(DELTA EQ 0.0) DELTA=0.78*RZB
IF(DTIL EQ 0.0) DTIL=1.1*DELTA +1.2*RVW
WRITE(6,200) RZB,RE
200 FORMAT(14HODENSITY RATIO .5X,12HREYNCGLOS NO/2E15*6) WRITE(6,201) DELTA,DTIL 201 FORMAT(6HODELTA,13X,4HDTIL /2E15*6) C 997 CONTINUE DO 995 I=1,NETA PI(I) = PD E(I) =0.0 995 CONTINUE C ** RANKIN-HUGONIOT RELATIONS ** C VD = -RZB TW = T(I) T(I) = T(I)/TD C ** STAGNATION POINT LIMIT QUANTITIES ** C DUD = DPHI + RZB*(1-OPHI) C NONDIMENSIONALIZING FACTORS AKNF = 1.8*778.28*TD *RZB/(R*RINF*UINF*UINF2) CPNF = 1.6*778.28*32.172*TD *2. /UINF2 C GUESSED F AND Z PROFILES C IF(KEEP .GT. 0) GO TO 9 N = NETA-2 FD = RZB/(2*DUD*DTIL) FW = -RVW*FD F(1) = FW DO 2 K=2,NETA F(K) = (FD-FW)*ETA(K) + FW 2 CONTINUE DD 3 I=1,N Z(I) = ETA(I+1)/DTIL 3 CONTINUE
C GUESSED T PROFILES
   IF(KEEP.GT.0)GOTO9
   IF(LT.GT.0) GO TO 11
   IF(RVW.GT.0)GOTO7
C NO BLOWING T PROFILE
   TWG1 = .1033
   DO6K = 2*NETA
   TP = TG1(K) + (T(1) - TWG1)
   T(K) = TP - (T(1) - TWG1) * ETA(K)
   6 CONTINUE
   GO TO 11
C BLOWING T PROFILE
   D08K = 2*NETA
   TP = TG2(K) + (T(1) - TWG2)
   T(K) = TP - (T(1) - TWG2) * ETA(K)
   8 CONTINUE
   GO TO 11
C ** INITIALIZE SHOCK LAYER PARAMETERS FOR VARIABLE STEP SIZE
   DO 810 I=NETA,60
   ETA(I) = 1.0
   T(I) = 1.0
   E(I) = 0.0
   PI(I) = PD
   MU(I) = 1.0
   CP(I) = CP(NETA)
\[ \begin{align*}
\text{AK}(I) &= \text{AK}(\text{NETA}) \\
\text{V}(I) &= \text{VD} \\
\text{F}(I) &= \text{FD} \\
\text{FC}(I) &= \text{FD} \\
\text{DO 810 } J &= 1, \text{NSP} \\
C(J, I) &= C(J, \text{NETA}) \\
\text{HS}(J, I) &= 1.0 \\
\text{810 CONTINUE} \\
\text{1000 CONTINUE} \\
\text{DO 223 } J &= 1, 60 \\
\text{DO 223 } K &= 1, \text{NE} \\
223 \text{ EC}(K, J) &= 1.0 \times 10^{-20} \\
\text{C} \\
\text{DO 2211 } I &= 1, \text{NSP} \\
C(I, I) &= \text{CWALL}(I) \\
221 \text{ CONTINUE} \\
\text{C----- CALCULATE AMW(N)} \\
\text{C} \\
\text{WAMW} &= 0.0 \\
\text{DO 25 } J &= 1, \text{NSP} \\
25. \text{ WAMW} &= \text{WAMW} + \text{CWALL}(J)/\text{SMW}(J) \\
\text{WAMW} &= 1.0/\text{WAMW} \\
26. \text{ AMW}(I) &= \text{WAMW} \\
\text{C} \\
\text{C} \\
\text{C----- CONVERT WALL AND SHOCK COMPOSITIONS TO AN ELEMENTAL BASIS} \\
\text{C} \\
\text{DO 331 } I &= 1, \text{NE} \\
\text{EC}(I, I) &= 0.0 \\
\text{EC}(I, \text{NETA}) &= 0.0 \\
\text{DO 331 } I &= 1, \text{NSP} \\
\text{FAC} &= \text{AA}(I, J) \times \text{AWT}(J)/\text{SMW}(I) \\
\text{FC}(I, I) &= \text{EC}(I, I) + \text{FAC} \times C(I, I) \\
33. \text{ EC}(I, \text{NETA}) &= \text{EC}(I, \text{NETA}) + \text{FAC} \times C(I, \text{NETA}) \\
331. \text{ ECWALL}(J) &= \text{EC}(J, 1) \\
\end{align*} \]
C
D034N=NETA*60
D034J=1*NE
34 EC(J,N)=EC(J,NETA)
C
C **** COMPUTE MUDZ AND RMDZ ****
C
AC = 8.129E-08*(TD**1.659)/(PI(1)*R*UINF)
D01623J=1,NETA
1623 D(J) = AC*(T(J)**1.659)
CALL ELRAT
CALL CHEMEQ (1,NETA)
MUDZ = 1.0
CALL PROPRRT (NSP,NETA,NETA)
MUDZ = MU(NETA)
RMDZ = RM(NETA)
CALL PROPRRT (NSP,1,NETA)
DTILS = .01
IF(IDERUG*EQ*0) RETURN
WRITE(6,4000) VD,U,PD
WRITE(6,4000) DELTA,DTIL,RZB,RE
4000 FORMAT(1H0,6E15.6)
203 FORMAT(6E12.0)
100 FORMAT(1X,9E14.6)
RETURN
END
SUBROUTINE MOMTM

C ------ THIS SUBROUTINE SOLVES THE MOMENTUM EQUATION AS A
C SECOND ORDER EQUATION AND A FIRST ORDER EQUATION ------

COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
COMMON /DEL/ DELTA,DTIL,DTILS
COMMON /FRSTRM/ UINF, RINF, UINF2, F, RE, LXI, ITM, IEM, NETA
COMMON /MAIM/KEEPS,MAXE,MAXM,MAXD,DEBUG,MCONV,ECONV,DCONV,LT,LAB
COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CFNF
COMMON /PROP1/PI(60),RHO(60), T(60),AMW(60),C (260),EC(5,60)
COMMON /PROP2/ M(60),RM(60),AK(60)
COMMON /PROP3/CPS(20,60),HS(20,60),CP (60),HM(60)
COMMON /RFLUX/ E(60),IRAD,ITYPE
COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTCTAL
COMMON /VECTOR/ CA(60),CB(60),CC(60),R(60)
COMMON /VEL/ F(60),FC(60),Z(60),V(60)
COMMON /WALL/RWW,PRW,TWOLD,FLUX(20),CWA(20),ECW(5)
COMMON /YL/ ETA(60),YON(60)
LOGICAL MCONV,ECONV,DCONV

C ------ INITIALIZED QUANTITIES ------

MCONV = .FALSE.
DTILS = DTIL
ITM = 1
N = NETA - 2
L = NETA - 1
AA3 = RZB*(1.0-RZB)*DPHI**2/DUD
DTILS2 = DTILS
IF(IEM.GT.3) DTIL = 5.0*(DTIL+DTILS2)

C

C

C ------ Z**A1*Z**A2*Z=A3
C COMPUTE A1,A2,A3
14 CONTINUE
C----- BOUNDARY CONDITIONS -----
C
RED = RE*DTIL
RED2 = 2.*RED*DTIL*UD
DTIL2 = DTIL*DTIL
FD = RZB/(2.*UD*DTIL)
FW = -RVW*FD
F(1) = FW
B(L) = 1./DTIL
ITER = 1
15 CONTINUE
II = 1
DO 20 I=1,N
DET=ETA(I+1)-ETA(I)
DFTN=ETA(I+2)-ETA(I+1)
D1 = DETN*(DETN*DET)
D2 = DETN*DET
D3 = DET*(DETN*DET)
RMP = DET*RM(I+2)/D1 + (DETN-DET)*RM(I+1)/D2 - DETN*RM(I)/D3
A1 = (RED2*F(I+1) + RMP)/RM(I+1)
A2 = -RED2*DTIL*Z(I)/RM(I+1)
A3 = -2.*RED*(A3/(RHO(I+1)*RM(I+1))
1 + DTIL2 *DUD*Z(I)**2/(2.*RM(I+1)))}
C
C-----CA*Z(N-1)+CB*Z(N)+CC*Z(N+1)=B
C
COMPUTE CA,CR,CC
CA(I) = (2* - A1*DETN)/D3
CR(I) = A1*(DETN-DET)/D2 - 2* /D2 + A2
CC(I) = (2* + A1*DET)/D1
B(I) = A3
II = I
20 CONTINUE
B(N)=B(N)-CC(N)/DTIL
C
CALL TRID (N)
C
--- INTEGRATE FIRST ORDER EQUATION ---
FC(1)=FW
SUM=FW + (B(1)+FW)*(ETA(2)-ETA(1))*DTIL/2.
FC(2)=SUM
DO 30 K=3,NETA
SUM=SUM+DTIL*(B(K-2)+B(K-1))*(ETA(K)-ETA(K-1))/2.
30 FC(K) = SUM
C
--- CHECK FOR CONVERGENCE ----
C
DO 40 K=2,NETA
PRCT=ABS((FC(K)-F(K))/F(K))
IF (PRCT.GT.FPRCT) GO TO 50
40 CONTINUE
GO TO 90
50 CONTINUE
ITER=ITER+1
DO 60 K=1,NETA
60 F(K)=FC(K)
DO 65 I=1,N
65 Z(I)=B(I)
IF (ITER.GE.MAXM ) GO TO 90
GO TO 15
90 CONTINUE
C
--- COMPUTE NEW DTIL ---
C
DTILC = (FD-FW)*DTIL/(F(NETA)-FW)
PRCT = ABS((DTIL-DTILC)/DTIL)
IF ( ITM.GT.MAXM) GO TO 160
ITM = ITM +1
IF (PRCT.LE.POTIL) GO TO 150
DTIL = DTIL +DDAMP*(DTILC-DTIL)
GO TO 14
CONTINUE

DTIL = DTIL + DDAMP*(DTILC - DTIL)
MCONV = .TRUE.

C CHECK MOMENTUM-ENERGY CONVERGENCE
PRCT = ABS((DTIL-DTILS)/DTILS)
IF(PRCT<=PDTIL) DCCNV = .TRUE.

CONTINUE

DO 170 K=1,NETA
170 V(K) = -FC(K)*DTIL*2/RHO(K)

C DEBUG OUTPUT
, IF(IDEBUG.EQ.0) RETURN
WRITE(6,102) ITER,ITM
102 FORMAT(10X,213/)
WRITE(6,100) DTIL,DTILC
WRITE(6,101)
101 FORMAT(6X,'ETA',12X,'F',12X,'FC',12X,'RHO',12X,'RM',12X,'VS',12X,
1 'V')
DO 120 K=1,NETA
VS=-FC(K)*DTIL*UINF*2/RHO(K)
WRITE(6,100) ETA(K),F(K),FC(K), RHO(K),RM(K),VS ,V(K)
120 FORMAT(1X,9E14*6)
CONTINUE

WRITE(6,103)
103 FORMAT(6X,'ETA',13X,'Z',13X,'B',12X,2HF')
DO 121 I=1,N
U=B(I)*DTIL
WRITE(6,100) ETA(I+1),Z(I),B(I),U
121 CONTINUE
RETURN
END
SUBROUTINE OUTPUT(N)

C
C ** ROUTINE TO PRINT SHOCK LAYER SOLUTION **
C
COMMON /ID/SP(20),EL(5)
COMMON /CONV/ FPRT,TPRT,DDAMP,TDAMP,PDTIL
COMMON /DEL/ DELTA,DIL,DILS
COMMON /FRSTRM/ U INF, R INF, UINF2, R, RE, LXI, ITM, IEM, NETA
COMMON /MAIN/KEEP,MAXE,MAXM,MAXD,DEBUG,MCONV,ECONV,DCONV,LT,IAB
LOGICAL MCONV,ECONV,DCONV
COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CFNF
COMMON /NUMBER/NSP,NNS,NE,NC
COMMON /PROP1/PI(60),RHC(60), T(60),AMW(60),C (20,60),EC(5,60)
COMMON /PROP2/ MU(60),RN(60), AK(60)
COMMON /PROP3/ CPS(20,60), HS(20,60), CP (60), H(60)
COMMON /RFLUX/ E(60), IRAD, ITYPE
COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
COMMON /SFLUX/QRI(7)
COMMON /VECTOR/ CA(60), CB(60), CC(60), B(60)
COMMON /VEL/ F(60), FC(60), Z(60), V(60)
COMMON /WALL/ RVW, PRV, TOLD, FLUX(20), CWALL(20), ECWALL(5)
COMMON /YL/ ETA(60), YOND(60)
COMMON /DD/ D(60)
COMMON /SP1/SS,TOL,NOBUG
DIMENSION BOUT(60),DQR(30)
REAL MU,MUDZ

DATA HEAD1/'WALL'/,HEAD2, '/*,HEAD3*,SHOC'/

C
C ** COMPUTE RADIATION FLUX IF UNCOUPLED PROBLEM **
C
IF (ITYPE .NE. 0) GOTO 20
IF (IRAD .EQ. 2 .AND. N .NE. 2) CALL TRANS(1)
IF (IRAD .NE. 1) CALL TRANS2

OUTP 10
OUTP 20
OUTP 30
OUTP 40
OUTP 50
OUTP 60
OUTP 70
OUTP 80
OUTP 90
OUTP 100
OUTP 110
OUTP 120
OUTP 130
OUTP 140
OUTP 150
OUTP 160
OUTP 170
OUTP 180
OUTP 190
OUTP 200
OUTP 210
OUTP 220
OUTP 230
OUTP 240
OUTP 250
OUTP 260
OUTP 270
OUTP 280
OUTP 290
OUTP 300
OUTP 310
OUTP 320
OUTP 330
OUTP 340
OUTP 350
20 IF(IRAD.EQ.2.AND.ITYPE.EQ.1) CALL EFLUX
   WRITE(6,203)
   203 FORMAT(1HI)
C
C ** COMPUTE Y COORDINATE **
C
   YOND(1) = 0.0
   SUM = 0.0
   DO 40 K=2,NETA
      DELTA = ETA(K) - ETA(K-1)
      SUM = SUM + DELTA*(1./RHC(K)+1./RHC(K-1))/2.
   END
   40 CONTINUE
   DELTA = YOND(NETA)
   DO 50 K=1,NETA
      YOND(K) = YOND(K)/DELTA
   END
C
C ** COMPUTE CONVECTIVE HEATING RATE **
C
   QC = -AK(1)*RINF*UINF*UINF2*(T(2)-T(1))/
         (*8E+779.28 *YCND(2)*DELTA*RZB)
   C BTU/FT**2-SEC
   CP = QC/88
C
C ** COMPUTE RADIATIVE FLUX TO SURFACE **
C
   IF(IRAD.EQ.1) GO TO 445
   DO 1100 K=2,NETA
      QR = QR + QUAD(YOND,E,K)
   END
   1100 CONTINUE
C
   QR = -QR*RINF*UINF2*UINF*DELTA/(685.*RZB)
IF (ITYPE.EQ.0) QR = -QRI(1)
CONTINUE
C BTU/FT**2-SEC
QRP = QR * 0.88
C ** COMPUTE DIFFUSIVE FLOW TO SURFACE **
C WATTS/CM**2
QD = 0.
DO 1768 I = 1, NSP
1768 QD = QD + HS(I,1) * (C(I,2) - C(I,1))
QD = - RHO(I) * D(I) * QD / (2. * DELTA * YOND(2))
QD = RINF * UINF * UINF2 * QD / (0.88 * 778.28)
C BTU/FT**2-SEC
QDP = 0.88 * QD
QTOTAL = QC + QR + QD
QTOTP = QTOTAL * 0.88
C ** DIMENSIONALIZE RHO, MU, P, AND E **
C DO 450 I = 1, NETA
RHO(I) = RHO(I) * RDZ
MU (I) = MU(I) * MUDZ
RM (I) = RM(I) * RMDZ
AK(I) = AK(I) / AKNF
E(I) = E(I) * RINF * UINF2 * UINF / (20866.0 * R * RZB)
CP(I) = CP(I) / CPNF
CONTINUE
C GO TO (1,2,3,4), N
C 1 WRITE (6,201) IEM
201 FORMAT (23H SOLUTION CONVERGED IN , I3, I11H ITERATIONS //)
GO TO 4
C 2 WRITE (6,202) IEM, MCONV, ECONV, DCONV
202 FORMAT (1H0, 37H INTERMEDIATE PRINT AT ITERATION NO. , I4, 10X,
1'MCONV='L4,5X,'ECONV='L4,5X,'DCONV='L4//')
GO TO 4
C
3 CONTINUE
C
4 CONTINUE
C
** PRINT SHOCK QUANTITIES AND HEATING RATE **
C
WRITE(6,204) DELTA,DTIL
204 FORMAT(1H0, 25X,9H DELTA = '1PE14.6,10X,7HD TIL = ',
1  E15.6)
C
WRITE (6,210) QC, QCP
210 FORMAT (1H0, 25X,5H QC = E15.6,2X,17H(WATTS/CM**2),
1  2X,1H='E15.6,2X,17H(BTU/FT**2 - SEC) )
WRITE(6,212) RZB, QR, QRP
212 FORMAT (1H0,6H RBl = 'F9.4,10X,5H QR = E15.6,2X,13H(WATTS/CM**2),
1  2X,1H='E15.6,2X,17H(BTU/FT**2 - SEC) )
WRITE(6,213) RVW, QD, QDP
213 FORMAT (1H0,5H RVH = 'F9.4,10X,5H QD = E15.6,2X,13H(WATTS/CM**2),
1  2X,1H='E15.6,2X,17H(BTU/FT**2 - SEC) )
C
WRITE(6,215) QTOTAL, QTOTP
215 FORMAT(1H0,16HTOTAL HEATING = E15.6,2X,13H(WATTS/CM**2),
1  2X,1H='E15.6,2X,17H(BTU/FT**2 - SEC) )
C
** PRINT Y/D, F AND T PROFILES **
C
WRITE(6,205)
205 FORMAT(1H0,7X, 4H ETA, 5X, 4HY/DZ, 8X, 2HF*, 8X, 3H RV, 8X ,
1  4H/TD, 4X, '13H E(WATTS/CM3),4X,2H V, 7X,12H V (FT/SEC) ,
2  5X,2H G,6X,12H H (STATIC), //)
FP = 0,0
NS=NSP
C
DO 100 I=1,NETA
C COMPUTE ENTHALPIES
HSTAT = 0.0
DO 99 J=1,NS
99 HSTAT = HSTAT + HS(J)*C(J)
G = HSTAT + V(I)**2
C
HEAD=HEAD2
IF (I .EQ. 1) HEAD=HEAD1
IF (I .EQ. NETA) HEAD=HEAD3
YDZ = YOND(I)
IF (I .EQ. NETA) FP = 1.0
RV = -FC(I)*DTIL
VS = V(I) *UINF
WRITE(6,208) HEAD,ETA(I),YDZ,FP,RV,T(I),E(I),V(I),VS,G,HSTAT
208 FORMAT(1H *A49 f6.3 l l0E12e3)
IF (I.LT.NETA) FP = Z(I)*DTIL
100 CONTINUE
C
** WRITE OUT SHOCK LAYER GAS PROPERTIES **
C
WRITE(6,44)
44 FORMAT(1H1.48X,28H-SHOCK LAYER GAS PROPERTIES-)
C
WRITE(6,206)
206 FORMAT(1H0.3X,3HETA,8X,4H Y/D,12X,2HP,12X,2H T,11X,3HRHO,11X,2HMU)

C
WRITE(6,207)
207 FORMAT(1H *27X.6H(AM),6X,13H (DEG.KEL.),12H (SLUGS/FT3),2X,1
28H(LBM/FT-SEC) (LBFT-SEC3/FT6),16H (BTU/FT-SEC-R),//)

C
DO 101 I=1,NETA
C
TS = T(I)*TD
WRITE(6,8) ETA(I), YOND(I), PI(I), TS, RHO(I), MU(I), RM(I), AK(I)

8 FORMAT(1H F7.4, 1P8E14.4)
9 FORMAT(1H F7.4, 1P7E14.4)

101 CONTINUE

** WRITE SPECIES MASS FRACTIONS **

WRITE(6,230)
230 FORMAT(1H1, 48X, 26H-SPECIES MASS FRACTIONS-

WRITE(6,231)
231 FORMAT(1H*14X, 3H 02, 11X, 2H N2, 11X, 3H O, 11X, 3H N, 11X, 3H O+,
1 11X, 3H N+, 11X, 3H E- ) )
DO 102 I=1, NETA
WRITE(6,8) ETA(I), C(1,I), C(2,I), C(3,I), C(4,I), C(5,I),
1 C(6,I), C(7,I)
102 CONTINUE

WRITE(6,230)
WRITE(6,233) (SP(I), I=8, 15)
233 FORMAT(2X, 4H ETA, 1X, 8(10X,A4)/)
WRITE(6,8) (ETA(I), (C(J,I), J= 8, 15), I=1, NETA)
WRITE(6,230)
WRITE(6,234) (SP(I), I=16, 20)
234 FORMAT(2X, 4H ETA, 7X, 3H CP, 5(11X, A4), 8X, 4H AMW, )
WRITE(6,9) (ETA(I), CP(I), (C(J,I), J=16, 20), AMW(I), I=1, NETA)

C NDIMENSIONALIZE
DO 1001 I=1, NETA
RHO(I) = RHO(I)/RDZ
MU(I) = MU(I)/MUDZ
RM(I) = RM(I)/RMDZ
E(I) = ((E(I)*R)/(RINF*UINF**3))*20866.0*RZB
CP(I) = CP(I)*CPNF
1001 AK(I) = AK(I)*AKNF
217 FORMAT(6E12.5)  
1000 CONTINUE  
C  
RETURN  
END  
OUTP2110  
OUTP2120  
OUTP2130  
OUTP2140  
OUTP2150
**PUNCH-OUT CARDS FOR RESTART**

**C**

```plaintext
SUBROUTINE PONCH

COMMON /CONV/ FRPRCT,TPRCT,DDAMP,TDAMP,PDTIL
COMMON/CONVI/HDAMP
COMMON /DEL/ DELTA,DTIL,DTILS
COMMON /FRSTRM/ UINF, RINF, UINF2, R, RE, LXI, ITM, IEM, NETA
COMMON /MAIM/KEEP, MAXE, MAXM, MAXD, IDEBUG, MCONV, ECONV, DCONV, LT, IAB
COMMON /NON/ RDZ, MUDZ, RMDZ, AKNF, HNF, CPNF
COMMON /NUMBER/ NSP, NFS, NE, NC
COMMON /PROP1/ PI(60), RHO(60), T(60), AMW(60), C(20,60), EC(5,60)
COMMON /PROP2/ MU(60), RM(60), AK(60)
COMMON /PROP3/ CPS(20,60), HS(20,60), CP(60), HM(60)
COMMON /RFLUX/ E(60), IRAD, IYPE
COMMON /RH/ DUD, DPHT, TD, RZB, PD, HD, HTCTAL
COMMON /VEL/ F(60), FC(60), Z(60), V(60)
COMMON /WALL/ RVW, PRW, TWOLD, FLUX(20), CWALL(20), ECWALL(5)
COMMON /YL/ ETA(60), YOND(60)
COMMON /TIT/TITLE(18)
COMMON /SPI/ SS, TDL, NDBG
REAL MU, MUDZ

*** PUNCH-OUT CARDS FOR RESTART ***

WRITE(7,566) TITLE, IEM
WRITE(7,1801) FRPRCT, TPRCT, DDAMP, TDAMP, PDTIL, HDAMP
WRITE(7,1801) DELTA, DTIL, DTILS
WRITE(7,1801) UINF, RINF, UINF2, R, RE, ITM, IEM, NETA
WRITE(7,1803) KEEP, MAXE, MAXM, MAXD, IDEBUG, MCONV, ECONV, DCONV, LT, IAB
PUNCH 1801, RDZ, MUDZ, RMDZ, AKNF, HNF, CPNF
WRITE(7,1804) NSP, NFS, NE, NC
WRITE(7,1801) (PI(J), RHO(J), T(J), J=1, NETA)
WRITE(7,1801) (AMW(J), J=1, NETA)
WRITE(7,1801) (C(I,J), J=1, NETA), I=1, NSP
WRITE(7,1801) (HM(J), J=1, NETA)
WRITE(7,1801) (E(J), J=1, NETA)
```

PONC 10  PONC 20  PONC 30  PONC 40  PONC 50  PONC 60  PONC 70  PONC 80  PONC 90  PONC 100
PONC 110  PONC 120  PONC 130  PONC 140  PONC 150  PONC 160  PONC 170  PONC 180  PONC 190
PONC 200  PONC 210  PONC 220  PONC 230  PONC 240  PONC 250  PONC 260  PONC 270  PONC 280
PONC 290  PONC 300  PONC 310  PONC 320  PONC 330  PONC 340  PONC 350
WRITE(7,1804)IRAD,ITYPE
PUNCH 1801, DUD*DPHI,TD,RZB,PD,HQ,HQTOTAL
WRITE(7,1801)(F(J),FC(J),Z(J),V(J),J=1,NETA)
PUNCH 1801, RWM,PRW,TWOLD
WRITE(7,1801)(CWALL(I),I=1,NSP)
WRITE(7,1801)(ECWALL(K),K=1,NE)
WRITE(7,1801)(ETA(J),YOND(J),J=1,NETA)
WRITE(7,715)NDEBUG,IRE,TOL
WRITE(7,1801)((EC(K,J),J=1,NETA),K=1,NE)
1801 FORMAT(6E13.5)
1802 FORMAT(5E12.5,3I3)
1803 FORMAT(5I5,3L3,2I5)
1804 FORMAT(4I4)
715 FORMAT(215,E15.6)
RETURN
END
SUBROUTINE GAS (KODE)

** THERMODYNAMIC AND TRANSPORT PROPERTIES OF AIR **

** REFERENCE NASA TR R-50 **

THE FOLLOWING PROPERTIES ARE CALCULATED

- TEMPERATURE AT WHICH PROPERTIES ARE WANTED (T) IN DEG R
- PRESSURE AT WHICH PROPERTIES ARE WANTED (P) IN LB/IN**2
- RATIO OF SPECIFIC HEATS (GAMMA) IN DIMENSIONLESS
- SPECIFIC HEAT AT CONSTANT PRESSURE (CP) IN BTU/LB-DEG R
- ABSOLUTE VISCOSITY (V) IN LB/FT-SEC
- PRANDTL NUMBER (PR) IN DIMENSIONLESS
- THERMAL CONDUCTIVITY (XK) IN BTU/FT-SEC-DEG R
- PRESSURE (P) IN ATMOSPHERES
- DENSITY (DEN) IN LB/FT**3
- ENTHALPY (H) IN BTU/LB
- ENTROPY (S) IN BTU/LB-DEG R
- COMpressibility (Z) IN DIMENSIONLESS
- SPEED OF SOUND (SOS) IN FT/SEC
- SPECIFIC HEAT AT CONSTANT VOLUME (CV) IN BTU/LB-DEG R
- ENTROPY (S) IN FT**2/SEC**2
- VELOCITY (VEL) IN FT/SEC
- PRESSURE (P) IN LBS/FT**2
- MACH NUMBER (M) IN DIMENSIONLESS

NOMENCLATURE

1=OXYGEN MOLECULES, 2=NITROGEN MOLECULES, 3=OXYGEN ATMOS
4=NITROGEN ATMOS, 5=OXYGEN IONS, 6=NITROGEN IONS
7=ELECTRONS

COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LX, ITM, IEM, NETA
COMMON /NON/RDZ, MUDZ, RMDZ, AKNF, HNF, CFNF
COMMON/PROP1/PI(60), RHO(60), TI(60), AMW(60), C (20, 60), CC(S, 60)
COMMON/PROP2/ MU(60), RM(60), AK(60)
COMMON/PROP3/CPS(20,60),HS(20,60),CPT(60),HM(60)
COMMON/RH/DUD,DPHI,TD,RZB,PD,HD,HTOTAL
COMMON/WALL/RW,PR,W,TWOLD,FLUX(20),CWALL(20),ECWALL(S)
REAL MU,MUDZ
LOGICAL MCONV,GCONV,SCONV
DATA GAS, /49721.7/

DO 2000 I=KODE,NETA
   T = T(I) * TD
   P = P(I)

THE FOLLOWING PART OF PROGRAM USES PRESSURE IN ATMOSPHERES
AND TEMPERATURE IN DEG K

ITER=0

** TEMPERATURE - ENTHALPY ITERATION **

900 CONTINUE
   ITER=ITER+1
   IF(TLT100) T=100
   A1=11390/T
   A2=16990/T
   A3=2270/T
   A4=3390/T
   A5=228/T
   A6=326/T
   A7=22800/T
   A8=48500/T
   A9=27700/T
   A10=41500/T
   A11=38600/T
   A12=58200/T
   A13=70.6/T

GAS 360
GAS 370
GAS 380
GAS 390
GAS 400
GAS 410
GAS 420
GAS 430
GAS 440
GAS 450
GAS 460
GAS 470
GAS 480
GAS 490
GAS 500
GAS 510
GAS 520
GAS 530
GAS 540
GAS 550
GAS 560
GAS 570
GAS 580
GAS 590
GAS 600
GAS 610
GAS 620
GAS 630
GAS 640
GAS 650
GAS 660
GAS 670
GAS 680
GAS 690
GAS 700
A14 = 188.9/T
A15 = 22000/T
A16 = 47000/T
A17 = 67900/T
A18 = 2270/(4*T)
A19 = TANH(A18)
A20 = 3390/(4*T)
A21 = TANH(A20)
TT = 1/T
TSQ = T**2
TSORT = T**.5
A22 = 112.2222/T
A23 = T/59000
A24 = T/113200
A25 = T/75400
AA1 = EXP(-A1)
AA2 = EXP(-A2)
AA3 = EXP(A3)
AA4 = EXP(A4)
AA5 = EXP(-A5)
AA6 = EXP(-A6)
AA7 = EXP(-A7)
AA8 = EXP(-A8)
AA9 = EXP(-A9)
AA10 = EXP(-A10)
AA11 = EXP(-A11)
AA12 = EXP(-A12)
AA13 = EXP(-A13)
AA14 = EXP(-A14)
AA15 = EXP(-A15)
AA16 = EXP(-A16)
AA17 = EXP(-A17)

C CALCULATING ENERGIES PER COMPONENT OF GAS MIXTURE ABOVE
C REFERENCE ENERGIES.

E1 = 2.5 + ((2.0 * AA1 * A1 + AA2 * A2) / (3.0 + 2.0 * AA1 + AA2)) + (A3 / (AA3 - 1.0))

GAS 710
GAS 720
GAS 730
GAS 740
GAS 750
GAS 760
GAS 770
GAS 780
GAS 790
GAS 800
GAS 810
GAS 820
GAS 830
GAS 840
GAS 850
GAS 860
GAS 870
GAS 880
GAS 890
GAS 900
GAS 910
GAS 920
GAS 930
GAS 940
GAS 950
GAS 960
GAS 970
GAS 980
GAS 990
GAS 1000
GAS 1010
GAS 1020
GAS 1030
GAS 1040
GAS 1050
\[ ET = 2.5 + \left( \frac{A4}{(AA4 - 1.0)} \right) \]
\[ E3 = 1.5 + \left( \frac{3 \times AA5 \times A5 + AA6 \times A6 + 5 \times AA7 \times A7 + AA8 \times A8}{(5.0 + 3.0 \times AA5 + AA6 + 5 \times AA7 + GAS)} \right) \]
\[ GAS 1060 \]
\[ E4 = 1.5 + \left( \frac{10 \times AA9 \times A9 + 6 \times AA10 \times A10}{(4 \times 10 \times AA9 + 6 \times AA10)} \right) \]
\[ GAS 1090 \]
\[ E5 = 1.5 + \left( \frac{10 \times AA11 \times A11 + 6 \times AA12 \times A12}{(4 \times 10 \times AA11 + 6 \times AA12)} \right) \]
\[ GAS 1100 \]
\[ E6 = 1.5 + \left( \frac{3 \times AA13 \times A13 + 5 \times AA14 \times A14 + 5 \times AA15 \times A15 + AA16 \times A16 + 5 \times AA17 \times A17)}{1.0 + 3.0 \times AA13 + 5.0 \times AA14 + 5.0 \times AA15 + AA16 + 5.0 \times AA17} \right) \]
\[ GAS 1120 \]
\[ E7 = 1.5 \]
\[ GAS 1130 \]

C TOTAL ENERGY PER COMPONENT OF GAS MIXTURE
\[ EN1 = E1 \]
\[ GAS 1150 \]
\[ EN2 = ET \]
\[ GAS 1160 \]
\[ EN3 = E3 + 29500 \times T \]
\[ GAS 1170 \]
\[ EN4 = E4 + 56600 \times T \]
\[ GAS 1180 \]
\[ EN5 = E5 + 18750 \times T \]
\[ GAS 1190 \]
\[ EN6 = E6 + 22540 \times T \]
\[ GAS 1200 \]
\[ EN7 = E7 \]
\[ GAS 1210 \]

C LOGS OF PARTITION FUNCTIONS
\[ TL1 = ALOG(T) \times 3 \times 5 \]
\[ GAS 1220 \]
\[ TL2 = ALOG(T) \times 2 \times 5 \]
\[ GAS 1230 \]
\[ E01 = TL1 + 11 + ALOG((3.0 + 2.0 \times AA1 + AA2)/(1.0 - (1.0/AA3))) \]
\[ GAS 1240 \]
\[ E02 = TL1 - 4.2 - ALOG((1.0 - (1.0/AA4))) \]
\[ GAS 1250 \]
\[ E03 = TL2 + 5 + ALOG((5.0 + 3.0 \times AA5 + AA6 + 5.0 \times AA7 + AA8)) \]
\[ GAS 1260 \]
\[ E04 = TL2 + 3 + ALOG((4.0 + 10.0 \times AA9 + 6.0 \times AA10)) \]
\[ GAS 1270 \]
\[ E05 = TL2 + 5 + ALOG((4.0 + 10.0 \times AA11 + 6.0 \times AA12)) \]
\[ GAS 1280 \]
\[ E06 = TL2 + 3 + ALOG((1.0 + 3.0 \times AA13 + 5.0 \times AA14 + 5.0 \times AA15 + AA16 + 5.0 \times AA17)) \]
\[ GAS 1290 \]
\[ E07 = TL2 - 14.24 \]
\[ GAS 1300 \]

C EQUILIBRIUM CONSTANS FOR CHEMICAL REACTIONS
\[ EK1 = -59000 \times T + 2.0 \times EQ3 - EQ1 \]
\[ GAS 1310 \]
\[ EK2 = -113200 \times T + 2.0 \times EQ4 - EQ2 \]
\[ GAS 1320 \]
\[ EK3 = -156800 \times T + EQ5 + EQ7 - EQ3 \]
\[ GAS 1330 \]
\[ EK4 = -168800 \times T + EQ6 + EQ7 = EQ4 \]
\[ GAS 1340 \]
\[ CCC = 79.9 \]
\[ GAS 1350 \]
\[ IF(EK1 \leq CCC) \] \[ EK1 = -79.9 \]
\[ GAS 1360 \]
\[ IF(EK2 \leq CCC) \] \[ EK2 = -79.9 \]
\[ GAS 1370 \]
\[ IF(EK3 \leq CCC) \] \[ EK3 = -79.9 \]
\[ GAS 1380 \]
IF(EK4 .LE. CCC) EK4 = -7.9

XK1 = EXP(EK1)
XK2 = EXP(EK2)
XK3 = EXP(EK3)
XK4 = EXP(EK4)
XK34 = 2*K3 .8*K4

EE1 = (-0.8 + (.64 + 8*(1.0 + ((4.*P)/XKI))) ** 0.5) / (2.0 + (1.0 + 4.*P/XKI))
EE2 = (-0.4 + (.16 + 3.84*(1.0 + (4.*P)/XK2))) ** 0.5) / (2.0 + (1.0 + 4.*P/XK2))
EE3 = 1.0 / ((1.0 + P/XK34) ** 0.5)

IF(EE1.EQ.19999) EE1 = 19999
IF(EE2.EQ.79999) EE2 = 79999
IF(EE3.EQ.99999) EE3 = 99999

C COMPRESSIBILITY (Z) DIMENSIONLESS
Z = 1.0 + EE1 + EE2 + 2.0 * EE3

C COMPONENT MOL FRACTIONS IN AIR
X1 = (2.0 - EE1) / Z
X2 = (8.0 - EE2) / Z
X3 = (2.0 + EE1 - 4.0 * EE3) / Z
X4 = (2.0 * EE2 - 1.6 * EE3) / Z
X5 = 4.0 * EE3 / Z
X6 = 1.6 * EE3 / Z
X7 = 2.0 * EE3 / Z
IF(X1 .LT. 0.0) X1 = 1.E-20
IF(X2 .LT. 0.0) X2 = 1.E-20
IF(X3 .LT. 0.0) X3 = 1.E-20
IF(X4 .LT. 0.0) X4 = 1.E-20
IF(X5 .LT. 0.0) X5 = 1.E-20
IF(X6 .LT. 0.0) X6 = 1.E-20
IF(X7 .LT. 0.0) X7 = 1.E-20

C ENERGY PER MOL OF INITIALLY UNDISSOCIATED AIR-DIMENSIONLESS
FR = Z *(X1*EN1 + X2*EN2 + X3*EN3 + X4*EN4 + X5*EN5 + X6*EN6 + X7*EN7)

C ENTHALPY PER INITIAL MOL OF AIR-DIMENSIONLESS
HR = ER + Z

C ENTHALPY PER INITIAL MOL OF AIR (H) IN BTU/LB
H = HR * T * 1.2348
IF(KODELENTETA) GO TO 1000
HRATOS.5*(H-HD)/H
AHR = ABS(HRATO)
IF(AHRLE0.0010) GO TO 999
IF(ITERLT.1) GO TO 203
TP=T
HP=HRATO
T = T *(1.0 - HRATO)
IF(ITERLE15) GO TO 900

203 CONTINUE
TS=T*(1.0-HRATO)
IF(HRATOTP.0.0) TS=.5*(T+TP)
TP=T
T=TS
HP=HRATO
IF(ITERLE15) GO TO 900
WRITE(6,200) T,H,T
CONTINUE

200 FORMAT(39HITEMPERATURE-ENTHALPY DID NOT CONVERGE /3E15.6)

C CALL OUTPUT(4)
STOP

999 CONTINUE
T0 = T

C 1000 CONTINUE
C ENTROPY PER INITIAL MOL OF AIR-DIMENSIONLESS
D1=E01+E1+1.0
D2=E02+E2+1.0
D3=E03+E3+1.0
D4=E04+E4+1.0
D5=E05+E5+1.0
D6=E06+E6+1.0
D7=E07+E7+1.0

C TOTAL ENTROPY
SR=Z*(X1*D1+X2*D2+X3*D3+X4*D4+X5*D5+X6*D6+X7*D7)-Z*(X1*ALOG(X1) +
1*X2*ALOG(X2)+X3*ALOG(X3)+X4*ALOG(X4)+X5*ALOG(X5)+X6*ALOG(X6)+X7*
\[2\log(x7) - z\log(p)\]

C ENTROPY PER INITIAL MOL OF AIR (S) IN BTU/LB-DEG R

\[S = 5r*0.0686\]

C SPECIFIC HEAT AT CONSTANT VOLUME-CV

\[Ff1 = 3*s + 2*s * A1 + A2\]
\[12*e + ((25*A3*A3)/(12 - A19*A19)**)2\]
\[Cv2 = 2*e_5 + ((25*A4*A4)/(2*A21) + (1 - A21*A21)**2)\]
\[Cv3 = 1 + 5*(3*A5*A5 + A6*A6 + A7*A7 + A8*A8)/((5 + 3*A8)**2)\]
\[15 + e_5*A7 + A8\]
\[Cv4 = 1.5 + (10*A9*A9 + A10*A10 + A10*A10)/((4 + 10*A9 + A8)**2)\]
\[1 - (E4 - 1.5)**2\]
\[Cv5 = 1 + 5*(10*A11*A11 + A12*A12 + A12*A12)/((4 + 10*A11 + A12)**2)\]
\[1 - (E5 - 1.5)**2\]
\[Cv6 = 1 + 5*(3*A13*A13 + A14*A14 + A15*A15 + A16*A16)*gas\]
\[1*A16*A16 + A17*A17**2)/(1 + 3*A13*A13 + A14*A14 + A15*A15 + A16*A16 + A17**2)\]
\[1E6 - 1.5)**2\]

C LOGARITHMIC DERIVATIVES

\[Ck1 = TT*(59000/E + 2*E - E1)\]
\[Ck2 = TT*(113200/E + 2*E - E1)\]
\[Ck3 = TT*(158000/E + T + E + E - E3)\]
\[Ck4 = TT*(168000/E + T + E + E - E4)\]
\[Ck34 = 2*Ck3 + 8*Ck4\]
\[P1 = Ck1 + T\]
\[P2 = Ck2 + T\]
\[P3 = Ck3 + T\]
\[P4 = Ck4 + T\]
\[Pk34 = 0.2*Pk3 + 0.8*Pk4\]

C PARTIAL DERIVATIVES REQUIRED FOR CP

\[De1p = (Pk1*E1*(1 + E1)*(E2 - E1))/((8 + 5 - E1))\]
\[De2p = (Pk2*E2*(1 + E2)*(E8 - E2))/((4 + 8 - E2))\]
\[De3p = 5*Pk34*E3*(1 - E3)**2\]
\[Dz1P = -De1P\]
\[Dz2P = -De2P\]

GAS 2110
GAS 2120
GAS 2130
GAS 2140
GAS 2150
GAS 2160
GAS 2170
GAS 2180
GAS 2190
GAS 2200
GAS 2210
GAS 2220
GAS 2230
GAS 2240
GAS 2250
GAS 2260
GAS 2270
GAS 2280
GAS 2290
GAS 2300
GAS 2310
GAS 2320
GAS 2330
GAS 2340
GAS 2350
GAS 2360
GAS 2370
GAS 2380
GAS 2390
GAS 2400
GAS 2410
GAS 2420
GAS 2430
GAS 2440
GAS 2450
\[ \text{C EQUATION FOR SPECIFIC HEAT AT CONSTANT PRESSURE} \]
\[ \text{CPR} = \text{CPF} + T*(DZX1P*(EN1+1)+DZX2P*(EN2+1)+DZX3P*(EN3+1)+DZX4P*(EN4+1)+DZX5P*(EN5+1)+DZX6P*(EN6+1)+DZX7P*(EN7+1)) \]
\[ \text{CP} = \text{CPR} \]
\[ \text{C SPECIFIC HEAT AT CONSTANT PRESSURE (CP) IN BTU/LB-DEG} \]
\[ \text{CP} = \text{CPF} \times 0.686 \]
\[ \text{C DENSITY (DEN) IN LB/FT}^3 \]
\[ \text{DEN} = 22.03703*P/(Z*T) \]
\[ \text{C **TRANSPORT PROPERTIES**} \]
\[ \text{C COLLISION CROSS SECTIONS} \]
\[ S2 = 31.4*1.0*E-16*(1+(12.5/T)) \]
\[ S2 = (S2/3.1415927)*2 \]
\[ S4 = 3.1415927*(S124)**2 \]
\[ S4 = (S12+SI4)/2 \]
\[ S7 = 5.40*1.0*E-1/TSQRT \]
\[ F = \text{ALOG}(1.042*1.0*E-7*TSQ*(P*777)**(-5)) \]
\[ S7 = 8.55644*1.0*E-6*1/TSQ*FI \]
\[ S4 = 3.1415927*(S14)**2 \]
\[ S24 = (S12+SI4)/2 \]
\[ S124 = (S12+S14)/2 \]
\[ S24 = 3.1415927*S124**2 \]
\[ SIP24 = 3.145927*SIP24**2 \]
\[ SF = 3.145927*SIP24**2 \]
\[ SF = (S12+SIP24)/2 \]
\[ SF = 3.145927*SIP24**2 \]
\[ \text{C COMPONENT MOL FRACTIONS FOR INDEPENDENT REACTIONS} \]
\[ F_1 = 1 + EE_1 \]
\[ F_2 = 1.2 + EE_2 \]
\[ F_3 = 1 + EE_3 \]
\[ X_1DD = (1.2 - EE_1) / F_1 \]
\[ X_2DD = 0.8 / F_1 \]
\[ X_3DD = 2 * EE_1 / F_1 \]
\[ X_2ND = (1.8 - EE_2) / F_2 \]
\[ X_3ND = 4 / F_2 \]
\[ X_4ND = 2 * EE_2 / F_2 \]
\[ X_4I = (1 - EE_3) / F_3 \]
\[ X_6I = EE_3 / F_3 \]

**C - MEAN FREE PATH RATIOS**

\[ SS_1 = S_2 / S_2 \]
\[ SS_2 = S_4 / S_2 \]
\[ SS_3 = S_7 / S_2 \]
\[ SS_4 = S_4 / S_2 \]
\[ F_{P10D} = X_{10I} + X_{20D} \times 0.660918 + X_{30D} \times 8164966 \]
\[ F_{P20D} = X_{10I} \times 1.032796 + X_{20D} \times 30D \times SS_1 \times 8528029 \]
\[ F_{P30D} = X_{10I} \times 1.154701 \times SS_1 + X_{20D} \times SS_1 \times 1.128152 + X_{30D} \times SS_2 \]
\[ F_{P2ND} = X_{20D} \times SS_1 \times 8164966 + X_{30D} \times SS_1 \times 8528029 \]
\[ F_{P3ND} = X_{20D} \times SS_1 \times 1.154701 + X_{40D} \times SS_2 \times X_{30D} \times SS_2 \times 1 \times 032796 \]
\[ F_{P4I} = X_{4I} \times SS_2 + X_6I \times SS_3 \]
\[ F_{P6I} = X_{4I} \times SS_2 + X_6I \times SS_3 \]
\[ F_{P7I} = X_{4I} \times SS_4 \times 1.414186 + X_6I \times SS_3 \times 1.414186 + X_6I \times SS_3 \]

**C - VISCOSITIES OF THE COMPONENTS FOR THE DIFFERENT REACTIONS**

\[ V_{10D} = 1.054093 \times X_{10D} \times 1 / F_{P10D} \]
\[ V_{20D} = 0.960133 \times X_{20D} \times 1 / F_{P20D} \]
\[ V_{30D} = 745356 \times X_{30D} \times 1 / F_{P30D} \]
\[ V_{2ND} = 0.960133 \times X_{2ND} \times 1 / F_{P2ND} \]
\[ V_{3ND} = 745356 \times X_{3ND} \times 1 / F_{P3ND} \]
\[ V_{4ND} = 6972167 \times X_{4ND} \times 1 / F_{P4ND} \]
\[ V_{4I} = 6572167 \times X_{4I} \times 1 / F_{P4I} \]
\[ V_{6I} = 6972167 \times X_{6I} \times 1 / F_{P6I} \]
\[ V_{7I} = 4.367848 \times 1 \times 0.52 \times X_{6I} \times 1 / F_{P7I} \]
VROD = V10D + V20D + V30D
VRND = V2ND + V3ND + V4ND
VRI = V4I + V6I + V7I
F4 = EE2/(E - EE1 + EE2)
F5 = 2*EE3/(E - EE2 + 2*EE3)
VR = VROD + (F4*(VRND - VROD)) + (F5*(VRI - VRND))

C TOTAL VISCOITY (V) IN LB/FT-SEC
V = VR * 9841838 * 1E-06 * TSQRT/(I + A22)

C CONDUCTIVITY DUE TO MOLECULAR COLLISIONS FOR DIFFERENT REACTIONS
G1 = 2105263*CV1 + .4736842
G2 = 2105263*CV2 + .4736842
G3 = 2105263*CV3 + .4736842
G4 = 2105363*CV4 + .4736842
G5 = 2105363*CV5 + .4736842
G6 = 2105363*CV6 + .4736842
XKNOD = (V10D * 9*G1) + (V20D * 9*028571 * G2) + (V30D * 1.8 * G3)
XKNND = (V2ND * 1.028571 * G2) + (V3ND * 1.8 * G3) + (V4ND * 0257143 * G4)
XKNI = (V4I * 2.057143 * G4) + (V6I * 2.057143 * G5) + (V7I * 32416 * 0 * G6)
XKN = XKNOD + (F4*(XKNND - XKNOD)) + (F5*(XKNI - XKNND))

C CONDUCTIVITY DUE TO CHEMICAL REACTIONS FOR THE DIFFERENT REACTIONS
G1 = 2105263*T*PK1**2/((SP24/(1.732051*S2)) + ((X30D + 2*X10D) * X10D))
G2 = 2105263*T*PK2**2/((SP24/(1.732051*S2)) + ((X4ND + 2*X2ND) * X2ND))
G3 = 2105363*T*PK3**2/((SP4*2*X3ND/(52*X4ND)) + (SP4*2*X3ND/(52*X4ND)))
G4 = 2105363*T*PK4**2/((5*SP4/S2) + (4.347826*1.0E-2*S47/S2))

PRN = .2105263 * CPR * VR / XKR
PRN = .2105263 * CPR * VR / XKR
PRW = PRN

C TOTAL THERMAL CONDUCTIVITY (XK) IN BTU/FT-SEC-DEG R
XK = XKR * (3206522*1.0E-6*TSQRT)/(1.0 + A22)

C PRANDTL NUMBER (PR) DIMENSIONLESS
PR = .2105263 * CPR * VR / XKR
IF (I.EQ. 1) PRW = PRN

PR = .2105263 * CPR * VR / XKR
IF (I.EQ. 1) PRW = PRN
FORM REQUIRED BY CALL STATEMENT  
** RHO UNITS SLUGS/FT**3  
** MU UNITS LBM/FT-SEC  
** RM UNITS LBF**2 SEC**3/FT**6  

```
MU(I) = V  
RHO(I) = DEN/32.174  
RM(I) = RHO(I)*MU(I)/32.174  
AK(I) = XK  
CPT(I) = CPF  
```

*** CALCULATE THE MEAN MOLECULAR WT. ***  

```
REAL = 25050*S*S/Z/SR  
AMW(I) = GASC/REAL  
```

MASS FRACTIONS  

```
C(1,I) = X1 *32.00/AMW(I)  
C(2,I) = X2 *28.00/AMW(I)  
C(3,I) = X3 *16.00/AMW(I)  
C(4,I) = X4 *14.00/AMW(I)  
C(5,I) = X5 *16.00/AMW(I)  
C(6,I) = X6 *14.00/AMW(I)  
C(7,I) = X7 *(1/820)*AMW(I)  
```

SPECIES ENTHALPY PER INITIAL MOLE OF AIR IN BTU/LB OF I  

```
HS(1,I) = (Z*X1*EN1/C(1,I) +Z)*T*12348  
HS(2,I) = (Z*X2*EN2/C(2,I) +Z)*T*12348  
HS(3,I) = (Z*X3*EN3/C(3,I) +Z)*T*12348  
HS(4,I) = (Z*X4*EN4/C(4,I) +Z)*T*12348  
HS(5,I) = (Z*X5*EN5/C(5,I) +Z)*T*12348  
HS(6,I) = (Z*X6*EN6/C(6,I) +Z)*T*12348  
HS(7,I) = (Z*X7*EN7/C(7,I) +Z)*T*12348  
```

2000 CONTINUE  

```
MUDZ = MU(NETA)  
RDZ = RHO(NETA)  
RMDZ = RM(NETA)  
```
C DO 40 I=KODE*NETA
C ** NONDIMENSIONALIZE RHO AND MU **
C RHO(I) = RHO(I)/RDZ
MU(I) = MU(I)/MUDZ
RM(I) =RM(I)/RMDZ
AK(I) = AK(I)*AKNF
CPT(I) = CPT(I)*CPNF
C NONDIMENSIONAL SPECIES ENTHALPY
HS(1,I) = HS(1,I)*HNF
HS(2,I) = HS(2,I)*HNF
HS(3,I) = HS(3,I)*HNF
HS(4,I) = HS(4,I)*HNF
HS(5,I) = HS(5,I)*HNF
HS(6,I) = HS(6,I)*HNF
HS(7,I) = HS(7,I)*HNF
C 40 CONTINUE
100 FORMAT(1X,9E14.6)
RETURN
END
SUBROUTINE FG2 (Y,RHOA,TK)
C--------
ORDER OF SPECIES ISO
C
C 1 2 3 4 5 6 7 8 9
HCN H2 H N2 N N+ O
C 10 11 12 13 14 15 16 17 18 19
C
C
C
COMMON/FOG/A!
DIMENSION Y(19),T1(5)
DIMENSION RHO(2),OK(16*2),PL(16.1O),RATES(3.16),EQK(16)
DATA R/82905/
DATA RATES/
DATA/82.05/
DATA RATES/
1 4352597E 02, 5000000E 00, 3572848E 05, 2683251E 02, 140
2 5000000E 00, 1761263E 05, 4835429E 02, 1500000E 01, 150
3 1131738E 06, 4272747E 02, 8200000E 00, 5193211E 05, 160
4 2866664E 02, 5000000E 00, 1575073E 06, 2876062E 02, 170
5 5000000E 00, 1675716E 06, 4684016E 02, 1000000E 01, 180
6 6632414E 05, 4357476E 02, 5000000E 00, 6038617E 05, 190
7 4369782E 02, 5000000E 00, 7045053E 05, 4369782E 02, 200
8 5000000E 00, 5886562E 05, 4588918E 02, 1000000E 01, 210
9 1297799E 06, 4374912E 02, 5000000E 00, 9561144E 05, 220
A 4367655E 02, 5000000E 00, 7799680E 05, 4368724E 02, 230
1 5000000E 00, 1333528E 06, 4369782E 02, 5000000E 00, 240
2 8303098E 05, 4369782E 02, 5000000E 00, 7296662E 05, 250
DIMENSION E1(95),E2(95),E3(34),E(16,7,2)
DATA E1/
DATA E1/
1 0.3530E 00, 0.1816E 01, 0.1727E 01, 0.1642E 01, 0.2321E 01, 290
2 0.2753E 01, 0.1675E 01, 0.2257E 01, 0.3458E 01, 0.2094E 01, 300
3 0.2028E 01, 0.3035E 01, 0.7810E 00, 0.2497E 01, 0.2132E 01, 310
4 0.7030E 00,-0.7681E-03,-0.3571E-02,-0.8059E-03,-0.2810E-03, 320
5 0.2250E-03,-0.3726E-03,-0.6017E-03,-0.2955E-02,-0.3852E-02, 330
6 0.2155E-02,-0.1370E-02,-0.4032E-02,-0.1175E-03, 0.6404E-04, 340
7 0.2840E-02,-0.1406E-02, 0.5153E-06, 0.1634E-05, 0.1344E-06, 350
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EQUVALENCE (E(16,6,1),E2(1))

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EQUVALENCE (E(15,5,2),E3(1))

DATA E3/
C
RHOA= DENSITY (LBM/FT3)

RHOB= .031085*RHOA
RHO(1)=.515362*RHOB
RHO(2)=RHO(1)*RHO(1)
X=0
DO 6 I=1, 19
6 X=X+Y(I)
   IF(ABS((TN-T)/TN)>.0001)20, 20, 10
10 T=TN
   T1(1) = T
   DO12 M=2, 4
12 T1(M) = T1(1)*T(M-1)
   T1(5) = ALOG(T1(1))
   RT = R*T
   L=1
   IF(T1(1)>600.0) L=2
   DO 18 I=1, L6
   QK(I,1)=T**RATES(2,I)* EXP(RATES(1,I)-RATES(3,I)/T)
   QK(I,2) = E(I,1,L)*TI(5)-E(I,2,L)*TI(1)/2.-E(I,3,L)*TI(2)/6.
   X-E(I,4,L)*TI(3)/12.-E(I,5,L)*TI(4)/20.+E(I,6,L)/TI(1)-E(I,7,L)
   EKQ(I) = EXP(-QK(I,2))
   QK(I,2) = QK(I,1)/ EKQ(I)
   IF(I.GT.2)QK(I,2) = RT*QK(I,2)
   CONTINUE
20 PL( 1, 1) = QK( 1, 1)*RHO(1)*Y( 12)
   IND = 0
   PL( 1, 2) = QK( 1, 1)*RHO(1)*Y( 1)
   PL( 1, 6) = QK( 1, 2)*RHO(1)*Y( 14)
\begin{align*}
& \text{PL}(1, 7) = QK(1, 2) \ast \text{RHO}(1) \ast Y(1, 7) \\
& \text{PL}(2, 1) = QK(2, 1) \ast \text{RHO}(1) \ast Y(10) \\
& \text{PL}(2, 2) = QK(2, 1) \ast \text{RHO}(1) \ast Y(6) \\
& \text{PL}(2, 6) = QK(2, 2) \ast \text{RHC}(1) \ast Y(9) \\
& \text{PL}(2, 7) = QK(2, 2) \ast \text{RHO}(1) \ast Y(3) \\
& \text{PL}(3, 1) = QK(3, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(3, 6) = 2 \ast QK(3, 2) \ast \text{RHO}(2) \ast Y(12) \ast X \\
& \text{PL}(3, 5) = QK(3, 1) \ast \text{RHO}(1) \ast Y(11) \\
& \text{PL}(3, 10) = QK(3, 2) \ast \text{RHO}(2) \ast Y(12) \ast Y(12) \\
& \text{PL}(4, 1) = QK(4, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(4, 6) = 2 \ast QK(4, 2) \ast \text{RHO}(2) \ast Y(10) \ast X \\
& \text{PL}(4, 5) = QK(4, 1) \ast \text{RHO}(1) \ast Y(9) \\
& \text{PL}(5, 1) = QK(5, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(5, 6) = QK(5, 2) \ast \text{RHO}(2) \ast Y(16) \ast X \\
& \text{PL}(5, 7) = QK(5, 2) \ast \text{RHO}(2) \ast Y(15) \ast X \\
& \text{PL}(5, 5) = QK(5, 1) \ast \text{RHO}(1) \ast Y(14) \\
& \text{PL}(5, 10) = QK(5, 2) \ast \text{RHO}(2) \ast Y(15) \ast Y(16) \\
& \text{PL}(6, 1) = QK(6, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(6, 6) = QK(6, 2) \ast \text{RHO}(2) \ast Y(16) \ast X \\
& \text{PL}(6, 7) = QK(6, 2) \ast \text{RHO}(2) \ast Y(13) \ast X \\
& \text{PL}(6, 5) = QK(6, 1) \ast \text{RHO}(1) \ast Y(12) \\
& \text{PL}(6, 10) = QK(6, 2) \ast \text{RHO}(2) \ast Y(13) \ast Y(16) \\
& \text{PL}(7, 1) = QK(7, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(7, 6) = QK(7, 2) \ast \text{RHO}(2) \ast Y(12) \ast X \\
& \text{PL}(7, 7) = QK(7, 2) \ast \text{RHO}(2) \ast Y(2) \ast X \\
& \text{PL}(7, 5) = QK(7, 1) \ast \text{RHO}(1) \ast Y(7) \\
& \text{PL}(7, 10) = QK(7, 2) \ast \text{RHO}(2) \ast Y(2) \ast Y(12) \\
& \text{PL}(8, 1) = QK(8, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(8, 6) = QK(8, 2) \ast \text{RHO}(2) \ast Y(10) \ast X \\
& \text{PL}(8, 7) = QK(8, 2) \ast \text{RHO}(2) \ast Y(7) \ast X \\
& \text{PL}(8, 5) = QK(8, 1) \ast \text{RHO}(1) \ast Y(8) \\
& \text{PL}(8, 10) = QK(8, 2) \ast \text{RHO}(2) \ast Y(7) \ast Y(10) \\
& \text{PL}(9, 1) = QK(9, 1) \ast \text{RHO}(1) \ast X \\
& \text{PL}(9, 6) = QK(9, 2) \ast \text{RHO}(2) \ast Y(10) \ast X
\end{align*}
PL(9, 7) = OK(9, 2) * RHO(2) * Y(3) * X
PL(9, 5) = OK(9, 1) * RHO(1) * Y(6)
PL(9, 10) = OK(9, 2) * RHO(2) * Y(3) * Y(10)
PL(10, 1) = OK(10, 1) * RHO(1) * X
PL(10, 6) = OK(10, 2) * RHO(2) * Y(10) * X
PL(10, 7) = OK(10, 2) * RHO(2) * Y(6) * X
PL(10, 5) = OK(10, 1) * RHO(1) * Y(17)
PL(10, 10) = OK(10, 2) * RHO(2) * Y(6) * Y(10)
PL(11, 1) = OK(11, 1) * RHO(1) * X
PL(11, 6) = OK(11, 2) * RHO(2) * Y(14) * X
PL(11, 7) = OK(11, 2) * RHO(2) * Y(2) * X
PL(11, 5) = OK(11, 1) * RHO(1) * Y(1)
PL(11, 10) = OK(11, 2) * RHO(2) * Y(2) * Y(14)
PL(12, 1) = OK(12, 1) * RHO(1) * X
PL(12, 6) = OK(12, 2) * RHO(2) * Y(2) * X
PL(12, 7) = OK(12, 2) * RHO(2) * Y(3) * X
PL(12, 5) = OK(12, 1) * RHO(1) * Y(4)
PL(12, 10) = OK(12, 2) * RHO(2) * Y(3) * Y(2)
PL(13, 1) = OK(13, 1) * RHO(1) * X
PL(13, 6) = 2 * OK(13, 2) * RHO(2) * Y(2) * X
PL(13, 5) = OK(13, 1) * RHO(1) * Y(3)
PL(13, 10) = OK(13, 2) * RHO(2) * Y(2) * Y(2)
PL(14, 1) = OK(14, 1) * RHO(1) * X
PL(14, 6) = OK(14, 2) * RHO(2) * Y(16) * X
PL(14, 7) = OK(14, 2) * RHO(2) * Y(5) * X
PL(14, 5) = OK(14, 1) * RHO(1) * Y(2)
PL(14, 10) = OK(14, 2) * RHO(2) * Y(5) * Y(16)
PL(15, 1) = OK(15, 1) * RHO(1) * X
PL(15, 6) = OK(15, 2) * RHO(2) * Y(2) * X
PL(15, 7) = OK(15, 2) * RHO(2) * Y(6) * X
PL(15, 5) = OK(15, 1) * RHO(1) * Y(18)
PL(15, 10) = OK(15, 2) * RHO(2) * Y(6) * Y(2)
PL(16, 1) = OK(16, 1) * RHO(1) * X
PL(16, 6) = OK(16, 2) * RHO(2) * Y(2) * X
PL(16, 7) = OK(16, 2) * RHO(2) * Y(18) * X

FG2 1410  
FG2 1420  
FG2 1430  
FG2 1440  
FG2 1450  
FG2 1460  
FG2 1470  
FG2 1480  
FG2 1490  
FG2 1500  
FG2 1510  
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FG2 1600  
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FG2 1660  
FG2 1670  
FG2 1680  
FG2 1690  
FG2 1700  
FG2 1710  
FG2 1720  
FG2 1730  
FG2 1740  
FG2 1750  

198
PL( 16, 5) = QK( 16, 1)*RHO(1)*Y(19)  FG2 1760
PL( 16, 10) = QK( 16, 2)*RHO(2)*Y(18)*Y( 2)  FG2 1770
GO TO (31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49) KFG2 1780
31 AA = PL( 11, 10) - PL( 11, 5)  FG2 1790
AII = AA - PL(11,1) - PL(11,1)  FG2 1800
GO TO 90  FG2 1810
32 BB= PL( 7, 6)+ PL( 7, 10)+ PL(11, 6)+ PL( 11, 10)  FG2 1820
BB=BB+ PL(12, 7)+ PL(12, 10)+2*PL(13, 6)+2*PL(13, 10)  FG2 1830
AA= PL( 7, 5)+ PL(11, 5)+ PL(12, 5)+2*PL(13, 5)  FG2 1840
AA=AA+ PL(14, 10)+ PL(15, 5)+ PL(16, 5)  FG2 1850
BB=BB+ PL(14, 1)+ PL(14, 5)+ PL(15,10)+ PL(15, 7)  FG2 1860
BB=BB+ PL(16,10)+ PL(16, 7)  FG2 1870
AII = AA - BB  FG2 1880
GO TO 90  FG2 1890
33 AA = PL( 9, 5)+ PL(12, 5)+ PL(13, 10)  FG2 1900
BB = PL( 9, 10)+ PL(12, 10)+ PL(13, 5)  FG2 1910
AA = AA - BB  FG2 1920
AII = AA - PL( 2, 6) - PL( 9, 6) - PL(12, 6)  FG2 1930
I = PL( 13, 1)  FG2 1940
GO TO 90  FG2 1950
34 AA = PL(12, 10)  FG2 1960
BB = PL(12, 5)  FG2 1970
AA = AA - BB  FG2 1980
AII = AA - PL(12, 1)  FG2 1990
GO TO 90  FG2 2000
35 BB = PL(14, 10)  FG2 2010
AA = PL(14, 5)  FG2 2020
AA = AA - BB  FG2 2030
AII = AA - PL(14, 6)  FG2 2040
GO TO 90  FG2 2050
36 AA = PL( 9, 10)+ PL(10, 5)+ PL(15, 5)  FG2 2060
BB = PL( 9, 5)+ PL(10, 10)+ PL(15, 10)+ PL(15, 6)  FG2 2070
AA = AA - BB  FG2 2080
AII = AA - PL( 2, 1) - PL( 9, 1) - PL(10, 6)  FG2 2090
GO TO 90  FG2 2100
37 AA = PL( 7, 10) + PL( 8, 5) FG2 2110
BB = PL( 7, 5) + PL( 8, 10) FG2 2120
AA = AA - BB FG2 2130
AII = AA - PL( 1, 6) - PL( 7, 1) - PL( 8, 6) FG2 2140
GO TO 90 FG2 2150
38 AA = PL( 8, 10) FG2 2160
BB = PL( 8, 5) FG2 2170
AA = AA - BB FG2 2180
AII = AA - PL( 8, 1) FG2 2190
GO TO 90 FG2 2200
39 AA = PL( 4, 10) FG2 2210
BB = PL( 4, 5) FG2 2220
AA = AA - BB FG2 2230
AII = AA - PL( 2, 7) - PL( 4, 1) FG2 2240
GO TO 90 FG2 2250
40 BB = PL( 2, 2) + 2*PL( 4, 6) + 2*PL( 4, 10) + PL( 8, 7) FG2 2260
BB = BB + PL( 8, 10) + PL( 9, 7) + PL( 9, 10) + PL( 10, 7) FG2 2270
AA = 2*PL( 4, 5) + PL( 8, 5) + PL( 9, 5) + PL( 10, 5) FG2 2280
BB = BB + PL( 10, 10) FG2 2290
AII = AA - BB FG2 2300
GO TO 90 FG2 2310
41 AA = PL( 3, 10) FG2 2320
BB = PL( 3, 5) FG2 2330
AA = AA - BB FG2 2340
AII = AA - PL( 3, 1) FG2 2350
GO TO 90 FG2 2360
42 BB = PL( 1, 2) + 2*PL( 3, 6) + 2*PL( 3, 10) + PL( 6, 1) FG2 2370
AA = 2*PL( 3, 5) + PL( 6, 10) + PL( 7, 5) FG2 2380
BB = BB + PL( 6, 5) + PL( 7, 7) + PL( 7, 10) FG2 2390
AII = AA - BB FG2 2400
GO TO 90 FG2 2410
43 AA = PL( 6, 5) FG2 2420
BB = PL( 6, 10) FG2 2430
AA = AA - BB FG2 2440
AII = AA - PL( 6, 6) FG2 2450
GO TO 90

44 AA = PL( 5, 10) + PL( 11, 5)
BB = PL( 5, 5) + PL( 11, 10)
AA = AA - BB
AII = AA - PL( 1, 7) - PL( 5, 1) - PL( 11, 7)

GO TO 90

45 AA = PL( 5, 5)
BB = PL( 5, 10)
AA = AA - BB
AII = AA - PL( 5, 6)

GO TO 90

46 AA = PL( 5, 5) + PL( 6, 5) + PL( 14, 5)
BB = PL( 5, 10) + PL( 6, 10) + PL( 14, 10)
AA = AA - BB
AII = AA - PL( 5, 7) - PL( 6, 7) - PL( 14, 7)

GO TO 90

47 AA = PL( 10, 10) - PL( 10, 5)
AII = AA - PL( 10, 1)

GO TO 90

48 AA = PL(15, 10) - PL(15, 5) + PL(16, 5) - PL(16, 10)
AII = AA - PL(15, 1) - PL(16, 6)

GO TO 90

49 AA = PL(16, 10) - PL(16, 5)
AII = AA - PL(16, 1)

PL( 1, 1) = Y( 1) * PL( 1, 1)
PL( 1, 6) = Y( 7) * PL( 1, 6)
PL( 2, 1) = Y( 6) * PL( 2, 1)
PL( 2, 6) = Y( 3) * PL( 2, 6)
PL( 3, 1) = Y( 11) * PL( 3, 1)
PL( 3, 6) = Y( 12) * PL( 3, 6) / 2
PL( 4, 1) = Y( 9) * PL( 4, 1)
PL( 4, 6) = Y( 10) * PL( 4, 6) / 2
PL( 5, 1) = Y( 14) * PL( 5, 1)
PL( 5, 6) = Y( 15) * PL( 5, 6)
PL( 6, 1) = Y( 12) * PL( 6, 1)
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<td>GO TO (51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69)</td>
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<tr>
<td>51</td>
<td>AA = PL( 1, 6) + PL( 11, 6)</td>
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<td>BB = PL( 1, 1) + PL( 11, 1)</td>
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<td>B = AA - BB</td>
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<td>GO TO 95</td>
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<tr>
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<td>AA = PL( 7, 6) + PL( 11, 6) + PL( 12, 6) + 2*PL( 13, 6)</td>
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<td>BB = PL( 7, 1) + PL( 11, 1) + PL( 12, 1) + 2*PL( 13, 1)</td>
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<td>AA = AA + PL( 14, 6) + PL( 15, 1) + PL( 16, 1)</td>
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<td>BB = BB + PL( 14, 1) + PL( 15, 6) + PL( 16, 6)</td>
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<td>B = AA - BB</td>
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<td>GO TO 95</td>
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<tr>
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<td>AA = PL( 2, 1) + PL( 9, 1) + PL( 12, 1) + PL( 13, 6)</td>
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<td>BB = PL( 2, 6) + PL( 9, 6) + PL( 12, 6) + PL( 13, 1)</td>
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<tr>
<td></td>
<td>B = AA - BB</td>
<td>3150</td>
</tr>
</tbody>
</table>
GO TO 95  

54 AA = PL(12, 6)  
BB = PL(12, 1)  
B = AA - BB  
GO TO 95  

55 AA = PL(14, 1)  
BB = PL(14, 6)  
B = AA - BB  
GO TO 95  

56 AA = PL(2, 6) + PL(9, 6) + PL(10, 1) + PL(15, 1)  
BB = PL(2, 1) + PL(9, 1) + PL(10, 6) + PL(15, 6)  
B = AA - BB  
GO TO 95  

57 AA = PL(1, 1) + PL(7, 6) + PL(8, 1)  
BB = PL(1, 6) + PL(7, 1) + PL(8, 6)  
B = AA - BB  
GO TO 95  

58 AA = PL(8, 6)  
BB = PL(8, 1)  
B = AA - BB  
GO TO 95  

59 AA = PL(2, 1) + PL(4, 6)  
BB = PL(2, 6) + PL(4, 1)  
B = AA - BB  
GO TO 95  

60 AA = PL(2, 6) + 2*PL(4, 1) + PL(8, 1) + PL(9, 1)  
BB = PL(2, 1) + 2*PL(4, 6) + PL(8, 6) + PL(9, 6)  
AA = AA + PL(10, 1)  
BB = BB + PL(10, 6)  
B = AA - BB  
GO TO 95  

61 AA = PL(3, 6)  
BB = PL(3, 1)  
B = AA - BB  
GO TO 95
62 AA = PL( 1, 6) + 2*PL( 3, 1) + PL( 6, 6) + PL( 7, 1)  FG2 3510
BB = PL( 1, 1) + 2*PL( 3, 6) + PL( 6, 1) + PL( 7, 6)  FG2 3520
B = AA - BB  FG2 3530
GO TO 95  FG2 3540
63 AA = PL( 6, 1)  FG2 3550
BB = PL( 6, 6)  FG2 3560
B = AA - BB  FG2 3570
GO TO 95  FG2 3580
64 AA = PL( 1, 1) + PL( 5, 6) + PL( 11, 1)  FG2 3590
BB = PL( 1, 6) + PL( 5, 1) + PL( 11, 6)  FG2 3600
B = AA - BB  FG2 3610
GO TO 95  FG2 3620
65 AA = PL( 5, 1)  FG2 3630
BB = PL( 5, 6)  FG2 3640
B = AA - BB  FG2 3650
GO TO 95  FG2 3660
66 AA = PL( 5, 1) + PL( 6, 1) + PL( 14, 1)  FG2 3670
BB = PL( 5, 6) + PL( 6, 6) + PL( 14, 6)  FG2 3680
B = AA - BB  FG2 3690
GO TO 95  FG2 3690
67 AA = PL( 10, 6)  FG2 3710
BB = PL( 10, 1)  FG2 3720
B = AA - BB  FG2 3730
GO TO 95  FG2 3740
68 AA = PL( 15, 6) + PL( 16, 1)  FG2 3750
BB = PL( 15, 1) + PL( 16, 6)  FG2 3760
B = AA - BB  FG2 3770
GO TO 95  FG2 3780
69 AA = PL( 16, 6)  FG2 3790
BB = PL( 16, 1)  FG2 3800
B = AA - BB  FG2 3810
95 IF (IND) 110, 101, 110  FG2 3820
101 IND = 1  FG2 3830
GAMMA = 0  FG2 3840
DO 102 I = 1, 16  FG2 3850
IF(I*GT.2)GAMMA = I* FG2 3860
Q = (RATES(2,I) + RATES(3,I)/T)/T FG2 3870
PL(I,1) = Q*PL(I,1) FG2 3880
Q = GAMMA/RT + Q - E(I,1,L)/T1(1) - E(I,2,L)/2 - E(I,3,L)*T1(1)/3FG2 3890
X* = E(I,4,L)*T1(2)/4 - E(I,5,L)*T1(3)/5 - E(I,6,L)/T1(2) FG2 3900
102 PL(I,6) = Q*PL(I,6) FG2 3910
C = B FG2 3920
GO TO 191 FG2 3930
110 RETURN FG2 3940
END FG2 3950
SUBROUTINE OUPPUT (IOUT)
COMMON/KKM/ALP(60),SVA(60),SDIFF(60),SAII(60),SB(60)
COMMON/FOG/AII,CWT,B,TOLD
COMMON/FRSTRM/UINF,RINF,UNF2,R,RE,LXI,ITM,IEM,NETA
COMMON/HR/DUD,DPHI,TD,RZB,PD,HD,HTOTAL
COMMON/YL/XXX(60),YOND(60)
COMMON/PROPI/PI(60),RHO(60),T(60),BMW(60),CM(20,60),CE(5,60)
DIMENSION Y(20,60)
EQUIVALENCE (CM(1),Y(1))
DIMENSION ETA(60)
EQUIVALENCE (NETA,NP),(PD,PRE),(YCND(1),ETA(1))

C
**** PRINT RESULTS OF SPECIES ITERATIONS ****
C
NS = 19
GO TO (1,2),IOUT
C OUTPUT CONVERGED RESULTS
1 CONTINUE
WRITE(6,61)
61 FORMAT(/4X.'PT.',17X*ETA%,13X.'DENSITY',9X.'TEMPERATURE',12X.'VELOC
ITY'/)
WRITE(6,71)(I,ETA(I),RHC(I) T(I),V(I),I=1,NP)
71 FORMAT(I7,4E20.7)
WRITE(6,50)
50 FORMAT(8X.'ETA%',9X.'N',10X.'N+',9X.'O',9X.'O+',9X.'E-',
X.'7X.C2H2',8X.'C3H',8X.'C4H')
DO 60 J=1,NP
60 FORMAT(8X.'ETA%',9X.'N',10X.'N+',9X.'O',9X.'O+',9X.'E-',
X.'7X.C2H2',8X.'C3H',8X.'C4H')
DO 60 J=1,NP
60 WRITE(6,40)ETA(J),(Y(I,J),I=11,19)
RETURN
END
SUBROUTINE COUPLE

C-----THIS SUBROUTINE SOLVES THE SPECIES AND ENERGY EQUATIONS

COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LXI, ITN, IEM, NETA
COMMON /CONV/ FPRT, TPRT, DDAMP, TDAMP, PDTIL
COMMON/CONV1/HDAMP
COMMON /DEL/ DELTA, DTIL, DTILS
COMMON /MAIN/ KEEP, MAXE, MAXN, MAXD, IDEBUG, MCONV, ECONV, DCONV, LT, IAB
COMMON /NON/RDZ, MUDZ, RMDZ, AKNF, HNF, CFNF
COMMON/NUMBER/NSP, NNS, NE, NC
COMMON/PROP1/PI(60), RHO(60), T(60), AMW(60), C(20,60), CE(5,60)
COMMON/PROP2/ MU(60), RM(60), AK(60)
COMMON/PROP3/CPS(20,60), HS(20,60), CP(60), HM(60)
COMMON/VECTOR/SUB(60), DIAG(60), SUP(60), B(60)
COMMON /RFLUX/ E(60), IRAD, IYPE
COMMON /V/ID/SP (20), EL(5)
COMMON /R/ DUD, DPHI, TD, RZB, PD, HD, HTOTAL
COMMON /SP2/B0, S(20), CMSHOCK(5)
COMMON /F/ F(60), FC(60), Z(60), V(60)
COMMON /VEL/ F(60), FC(60), Z(60), V(60)
COMMON /WALL/RW, PWR, TW, RV, TWOLD, FLUX(20), CWALL(20), ECWALL(5)
COMMON /Y/ ETA(60), YOND(60)
COMMON /OLD/ TOLD(60), EOLD(60), RHCS(60)
COMMON/DD/D(60)
DIMENSION RHOLD(60)
      REAL MU, MUDZ
      LOGICAL MCONV, ECONV, DCONV
      COMMON/NETI/NETA1, NETA2
      COMMON/KKB/RHOA, TA, VA, YA(19)
      COMMON/FOG/AII, BI, CI, TOLD1
      COMMON/IT/AC
      COMMON/CK/ISN(20), MWT(19)
      REAL MWT
      DIMENSION Y(20,60), SY(20,60)
      DIMENSION SACI(19,60)
DIMENSION RED (60),RES(60),RET(60)
DATA NS,SYNCH,SPER,TMCH/19.50,80.01/
C
C------INITIALIZE
C
NETA1 = NETA - 1
NETA2 = NETA - 2
ECONV = .FALSE.
ITER = 0
DO 10 J=1,NETA
10 TOLD(J) = T(J)
AC = 8.128E-08*(TD**1.659)/(PI(1)**R*UINF)
AR = R/UINF
C ** COMPUTE THE Y COORDINATE **
YOND(1) = 0.0
SUM = 0.0
DO 39 K=2,NETA
DETA = ETA(K) - ETA(K-1)
SUM = SUM +DETA*(1./RHC(K) +1./RHO(K-1))/2.0
YOND(K) = DTIL *SUM
39 CONTINUE
DELTA = YOND(NETA)
DO 49 K=1,NETA
YOND(K) = YOND(K)/YOND(NETA)
49 CONTINUE
IF(IAB.NE.0)GO TO 528
CALL SPECIE
CALL PROPRIT(NSP,1,NETA)
C **** COMPUTE FLUX DIVERGENCE ****
528 IF(IRAD.EQ.3.AND.ITYPE.EQ.1)CALL EFLUX
IF(IRAD.EQ.3.AND.ITYPE.EQ.0)CALL LRAD
TOLD1 = 0.
C
RDZ = DENSITY AT SHOCK (SLUGS OF M / FT**3)
RHOD = RDZ*32.174
C
RHOD = DENSITY AT SHOCK (LBM OF M / FT**3)
**CALCULATE DIFFUSION COEFFICIENT**

```fortran
110 DO120 J = 1, NETA
120 D(J) = AC*(T(J)**19659)
130 CALL PROPT (NSP, 1, NETA)

DX1 = ETA(J) - ETA(1)
DO200 J = 2, NETA1
DX = ETA(J + 1) - ETA(J)
J1 = J - 1
C013 = 2*RHO(J)*AK(J)/(DTIL*CP(J))
C014 = - RHO(J)*V(J)
C015 = (C1(DXDXI)*RHO(J+1)*AK(J+1)/CP(J+1) + C2(DXDXI)*RHO(J)*AK(J)/CP(J) + C3(DXDXI)*RHO(J-I)*AK(J-I)/CP(J-1))*2./DTIL
CON4 = 2*RHO(J)*V(J)*V(J)*(C1(DXDXI)*V(J+1) + C2(DXDXI)*V(J) + C3(DXDXI)*V(J-I))
CON5 = 2.*DTIL*E(J)/RHO(J)
CON6 = 0.
CON7 = 0.
CON8 = 0.
DO2023 I = 1, NSP
CON6 = CON6 + HS(I,J)*(C4(DXDXI)*C(I,J+1) + C5(DXDXI)*C(I,J))
X C6(DXDXI)*C(I,J-1))
CV = (C1(DXDXI)*C(I,J+1) + C2(DXDXI)*C(I,J))
X C3(DXDXI)*HS(I,J-1))
CON7 = CON7 + HS(I,J)*CV
C018 = C018 + CV*(C1(DXDXI)*HS(I,J+1) + C2(DXDXI)*HS(I,J) + C3(DXDXI)*HS(I,J-1))

2023 CONTINUE
CV = (2*RHO(J)*AK(J)/CP(J) - RHO(J)*RHO(J)*D(J))/DTIL
C016 = CON6*CV
CD = (C1(DXDXI)*RHO(J+1)*RHO(J+1)*D(J+1) + C2(DXDXI)*RHO(J)*RHO(J)*D(J+1) + C3(DXDXI)*RHO(J-1)*RHO(J-1)*D(J-1))/DTIL
C017 = CON7*(C015 - CD)
```
CO18 = CO18*CV
SUB(J1) = CO13
DIAG(J1) = CO14 + CO15
SUP(J1) = 0
B(J1) = CON5 + CON4 + CO17 + CO18 + CO16
200 DX1 = DX
CALL SOLVE (HM(1)*HM(NETA))
C-------
CHECK FOR CONVERGENCE
IF (IDERUG.EQ.0) GO TO 249
DO1532 K1 = 1, NETA2
    KK = K1 + 1
1532 WRITE (6, 1533) K1, ETA(KK)*HM(KK)*B(K1)
1533 FORMAT (1X, I10, F15.4, 2E20.6)
249 DO 250 J = 2, NETA1
    SRCT = (B(J-1) - HM(J))/HM(J)
    PRCT = ABS(SRCT)
    IF (PRCT.GT.TPRCT) GO TO 260
250 CONTINUE
GO TO 300
260 ITER = ITER + 1
DO 270 J = 2, NETA1
    SRCT = (B(J-1) - HM(J))/HM(J)
    SAP = HDAMP*SRCT
    IF (ABS(SAP).GT.TMCH) GO TO 1618
    ZIP = SAP
    GO TO 1619
1618 ZIP = TMCH*ABS(SAP)/SAP
1619 HM(J) = (1+ZIP)*HM(J)
    IF (HM(J).LE.HM(1)) HM(J) = 1.0001*HM(1)
    IF (HM(J).GT.1.0) HM(J) = .9999
270 CONTINUE
C
C........................ SOLVE FOR TEMPERATURE ........................
C
DO 818 J = 1, NETA
818 RED(J) = T(J)
     DO 756 J=2, NETA1
     B(J-1) = HM(J)
     ITEB = 0
     751 CALL PROPRN (NSPJ,J,J)
     DTT = (B(J-1) - HM(J))/CP(J)
     T(J) = T(J) + DTT
     DTT = DTT/T(J)
     ITEB = ITEB + 1
     IF (ITEB.GT.20) GO TO 752
     GO TO 754
     752 WRITE (6,753) J, DTT
     753 FORMAT (1X, 'TEMPERATURE AT THE ', I3, 'TH POINT DOES NOT CONVERGE',
                'CHANGE IN TEMPERATURE=', E20.6)
                  STOP

C
     754 IF (ABS(DTT).GT.0.01O) GO TO 751
     756 CONTINUE
     DO 9023 J=2, NETA1
     SRC1 = (T(J) - RED(J))/RED(J)
     SAP = TDAMP*SRC1
     IF (ABS(SAP).GT.TMCH) GO TO 9021
     ZIP = SAP
     GO TO 9022
     9021 ZIP = TMCH*ABS(SAP)/SAP
     9022 T(J) = (1.0 + ZIP)*RED(J)
     IF (T(J).LT.T(1)) T(J) = T(1)
     IF (IDEGE.EQ.0) GO TO 889
     WRITE (6, 817) (J*RED(J), T(J), J=1, NETA)
     817 FORMAT (1X, I5, 20X, 2F20.6)
     CONTINUE

C
     889 IF (ITER.EQ.MAXE) GOTO 300
     IF (IAB) 891, 891, 892
891 CALL SPECIE
    GO TO 110
892 CALL ELRAT
    CALL CHEMEQ (1,NETA)
    GO TO 110
300 CONTINUE
    IF (ITER.LT.MAXE) ECONV=.TRUE.
    DO 320 J=2,NETA1
        T(J) = T(J) + .35*(TOLD(J) - T(J))
        SRCT = (T(J) - TOLD(J))/TOLD(J)
    C IF (ABS(SRCT)*GT.TMCH) T(J) = TOLD(J) + TMCH*SRCT*TOLD(J)/ABS(SRCT)
320 CONTINUE
    RETURN
    END
SUBROUTINE ELRAT

COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LXI, ITM, IEN, NETA

COMMON /PROP1/ PI(60), RHO(60), T(60), AMW(60), C(20, 60), CE(5, 60)

COMMON /MAIM/ KEEP, MMAX, MMD, IDEBUG, MCONV, ECONV, DCONV, LT, IAB

COMMON /T/ AC

COMMON /NUMBER/ NSP, NE, NC

COMMON /YL/ ETA(60), YOND(60)

COMMON /NETI/ NETAI, NETA2

COMMON /VECTOR/ SUB(60), DIAG(60), SUP(60), B(60)

COMMON /DEL/ DELTA, DTIL, DTILS

COMMON /VEL/ F(60), FC(60), Z(60), V(60)

COMMON /VEL/ F(60), FC(60), Z(60), V(60)

C------ SOLVE ELEMENT CONSERVATION EQUATIONS -------

CE(1, NETA) = 1E-03
CE(2, NETA) = 1E-03

DO 116 K = 1, NE

DX1 = ETA(2) - ETA(1)

DO 106 J = 2, NETA1

DX = ETA(J+1) - ETA(J)

J1 = J - 1

SUB(J1) = RHO(J) * RHC(J) * D(J) / (DTIL * DTIL)

DIAG(J1) = (C1(DX, DX1) * RHO(J+1) * RHO(J+1) * D(J+1) + C2(DX, DX1) * XRHO(J) * RHO(J) * D(J) + C3(DX, DX1) * RHO(J-1) * RHO(J-1) * D(J-1)) - XRHO(J) * RHO(J) * V(J) / (DTIL * DTIL)

SUP(J1) = 0.

B(J1) = 0.

106 DX1 = DX

CALL SOLVE (CE(K, J), CE(K, NETA))

DO 116 J = 2, NETA1

116 CE(K, J) = B(J-1)

DO 117 J = K, 1, 5

117 CE(K, J) = CE(K, J+1)

IF (IDEBUG.EQ.0) GO TO 11

WRITE(6, 117) (J, CE(K, J), K = 1, 5), J = 1, NETA)
117 FORMAT(1X, 15, ZE20.7)
11 RETURN
END
SUBROUTINE SPECIE

C-----STAGNATION LINE SOLUTION OF SPECIES CONTINUITY EQUATION (SPC4)

C-------ORDER OF SPECIES ISO

C

C C0 C C2 C3 C+ C2H CN
C 1 2 3 4 5 6 7
C HCN H2 H N2 N N+ 0
C 3 9 10 11 12 13 14
C 0+ E- C2H2 C3H C4H

COMMON/COT/A1,CS
COMMON/N/NP1,NP2,NP3
COMMON/K/KB/RHA,TA,YA(19)
COMMON/KKM/ALP(#60),SVA(#60)
COMMON/FOG/AII,TOLD
COMMON/SAVE/SSUB(#60),SDIAG(#60),SSUP(#60),S(#60),E(#60)
DIMENSION IDEN(#19)

C* * * * * * * * * * * * * * * * * * * * SPEC 100
COMMON /DEL/ DELTA,DTIL,DTILS
COMMON/FRSTRM/ U INF, RINF, UINF2, F, RE, LXI, ITM, IEM, NETA
COMMON/PROPI/PI(#60),RHA(#60), T(#60),BMW(#60),CM(#20,60),CE(#5,60)
COMMON/RH/DUD,DPMI,TD,RZB,PD,HO,HTCTAL
COMMON/YL/XXX(#60),YOND(#60)

XXX IS ETA IN MAIN

COMMON/MAIM/KEEP,MAXM,MAXD,IDE BUG,MCONV,ECONV,DCONV,LT,IAB
COMMON/VECTOR/ CA(#60),CB(#60),CC(#60),ALT(#60)
COMMON/VEL/F(#60),FC(#60),Z(#60),V(#60)
COMMON/NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CNF
COMMON/NUMBER/NSP,NNS,NE,NC
COMMON/CK/ISN(#20),MWT(#19)

C* * * * * * * * * * * * * * * * * * * * SPEC 170
REAL MWT
DIMENSION Y(#20,60)
COMMON/SIS/SY(#20,60)
EQUIVALENCE (CM(1),Y(1))
DIMENSION ETA(#60)
EQUIVALENCE (NETA, NP), (PD, PRE), (YCND(1), ETA(1))
DIMENSION SUB(60), DIAG(60), SUP(60)
EQUIVALENCE (CA(1), SUB(1)), (CB(1), DIAG(1)), (CC(1), SUP(1))
DATA NS, SYMCH, SPER/19, 50, 80/
LOGICAL MCONV, ECONV, DCONV
C RDZ = DENSITY AT SHOCK (SLUGS OF M/FT**3)
      RHOD = RDZ*32.174
C RHOD = DENSITY AT SHOCK (LBM OF M/FT**3)
ISIFI=0
TOL2 = .02
TOL1 = 0.250000*TOL2
TOL3 = 2.0*TOL2
TOL4 = 4.0*TOL2
NID=2
NIT=1
IT=0
TOLD=0.
C NP=TOTAL NUMBER OF PROFILE POINTS
C PRE = STATIC PRESSURE (LBF/FT2)
C
NP1=NP - 1
NP2=NP - 2
NP3=NP - 3
C********** DIMENSIONALIZE
DO500I=1, NP
RHO(I) = RHO(I)*RHOD
T(I) = T(I)*TD
50 V(I) = V(I)*UINF
C ETA=Y(FT)
C RHO = DENSITY (LBM/FT3)
C T = TEMPERATURE PROFILE (OK)
C V = VELOCITY PROFILE (FT/SEC)
C NS=NO. OF SPECIES
C MWT=MOLECULAR WEIGHTS
C Y = MASS FRACTIONS
DO111I=1, NSP
DO111 J=1, NP
111 SY(I,J) = Y(I,J)
DO112 I=1, NP
DO112 J=1, NP
112 Y(I,J) = SY(ISN(I), J)
CALL OUTPUT(I)
DO100 I=1, NP
DO100 J=1, NP
100 Y(I, J) = Y(I, J)/MWT(I)
C Y = MOLES OF I/MASS OF MIXTURE
DO1971 J=1, NP
DO1971 K=1, NP
1971 SY(K, J) = Y(K, J)
C PATM=PRESSURE IN ATMOSPHERES
AC=8.128E-08
AC=AC/PRE
C---------CALCULATE DIFFUSION COEFFICIENT(DIFF)
DO170 J=1, NP
170 SDIFF(J) = AC*(T(J)**1.659)
C FIFF=(FT2/SEC)
C********COMPUTE PART OF THE ELEMENTS OF THE TRIO MATRIX********
DXI=ETA(2)-ETA(1)
DO1530 J=2, NP1
DX=ETA(J+1)-ETA(J)
SVA(J) = -V(J) + (C1(DX, DX1)*RHC(J+1)*SDIFF(J+1) + C2(DX, DX1)*RHO(J)
XJ)*SDIFF(J) + C3(DX, DX1)*RHC(J-1)*SDIFF(J-1)/RHO(J)
A = SDIFF(J)*C6(DX, DX1) + SVA(J)*C3(DX, DX1)
G = SDIFF(J)*C5(DX, DX1) + SVA(J)*C2(DX, DX1)
C = SDIFF(J)*C4(DX, DX1) + SVA(J)*C1(DX, DX1)
IF(J EQ 2) A1=A
IF(J EQ NP1) CS=C
IF(J EQ NP1) GO TO 1520
SSUP(J-1) = C
1520 SDIAG(J-1) = G
IF(J EQ 2) GO TO 1530
SSUB(J-2)=A
1530 DX1=DX

C********
DO321 I=1, NS
321 IDEN(I)=0

C********* OVERALL ITERATION LOOP **********
120 IT=IT+1
YMCH=SYMCH
PER=SPER
IF (IT*LT*21) GO TO 1181
1175 YMCH=10
1181 CONTINUE

C********* SPECIES ITERATION LOOP **********
DO200 I=1, NS
IF (IDEN(I).GE.4) GO TO 200
IDEN(I)=4
DO127 J=2, NPI
AMW=0
DO126 K=1, NS
126 AMW=AMW+Y(KJ)
AMW=1/AMW
DO127 K=1, NS
127 RHO(J)=.7608*PRE*AMW/T(J)

C********* COMPUTE REACTION RATE **********
DO550 J=2, NPI
JJ=J-1
DO530 L=1, NS
530 YA(L)=Y(L,J)
CALL FG2 (YAS.RHO(J),T(J),I)
SAII(JJ)=AIJ*DELTA
SB(JJ)=B*DELTA
3923 CONTINUE

C********
C********* COMPUTE ELEMENTS OF TRID. MATRIX AND SOLVE **********
DO1010 J=1, NPI
JJ=J+1
DIAG(J) = SDIAG(J) + SAII(J)
IF(J .EQ. NP2) GO TO 1010
SUB(J) = SSUB(J)
SUP(J) = SSUP(J)
1010 ALT(J) = SAII(J) * Y(I, JJ) - SB(J)
ALT(1) = ALT(1) - AI * Y(I, I)
ALT(NP2) = ALT(NP2) - CS * Y(I, NP)
CALL TRID(NP2)
DO 1080 J = 2, NP1
1080 ALP(J) = ALT(J - 1)
C*****
   IF(I .NE. 1) GO TO 2694
   IF(I .NE. 13) GO TO 2691
   DO 2690 JJ = 2, NP1
2690 Y(I, JJ) = ALP(JJ)
   IF(I .NE. 15) GO TO 2694
   DO 2692 JJ = 2, NP1
2692 Y(I, JJ) = ALP(JJ)
2694 CONTINUE
128 DO 130 J = 2, NP1
   ABD = (ALP(J) - Y(I, J)) / Y(I, J)
   AR = ABS(ABD)
   IF(ABS(Y(I, J)) .LT. 1.E-04 .AND. ABS(ALP(J)) .LT. 1.E-04) GO TO 1344
   IF(IDEN(I) .LT. 4) GO TO 6010
   IF(AB .GT. TOL1) IDEN(I) = 3
6010 IF(IDEN(I) .LT. 3) GO TO 6020
   IF(AB .GT. TOL2) IDEN(I) = 2
6020 IF(IDEN(I) .LT. 2) GO TO 6030
   IF(AB .GT. TOL3) IDEN(I) = 1
6030 IF(IDEN(I) .LT. 1) GO TO 6040
   IF(AR .GT. TOL4) IDEN(I) = 0
6040 CONTINUE
1344 CONTINUE
   SAP = PER * ABD
   IF(ABS(SAP) .GT. YMCH) GO TO 1618
ZIP=SAP
1618 ZIP=YMCH*ABS(SAP)/SAP
1619 CONTINUE
Y(I,J)=(1+ZIP)*Y(I,J)
130 CONTINUE
200 CONTINUE
IF(IT<LT.NIT)GO TO 374
IF(IDEBUG.EQ.0)GO TO 823
WRITE(6,1463)(I,IDENT(I),I=1,NS)
1463 FORMAT(6(4X.I3.2X,=*I5v4X))
823 DO373 I=1,NS
373 IDENT(I)=0
374 CONTINUE
C
IF(IT.NE.NIT)GO TO 376
DO375 I=1,NS
375 CONTINUE
GO TO 210
376 IF(IT<LT.NIT)GO TO 3334
NIT=NIT+5
NID=NIT-4
IF(IDEBUG.EQ.0)GO TO 3334
WRITE(6,218)IT,YMCH
218 FORMAT(/10X,'ITERATION NUMBER*','I10.5X,'YMCH*','F15.6/)
C
CALL OUTPUT (2)
3334 CONTINUE
GO TO 120
210 DO192 J=1,NP
AMW = 0.
DO191 I=1,NS
192 AMW = AMW + Y(I,J)
193 BMW(J) = 1./AMW
DO191 J=1,NS
DO191 J=1,NS

191 Y(I,J) = Y(I,J)*MWT(I) SPEC2110
C CALL OUPPUT (I) SPEC2120
C******** NON-DIMENSIONALIZE SPEC2130
D051 =1,NP SPEC2140
RHO(I) = RHO(I)/RHOD SPEC2150
T(I) = T(I)/TD SPEC2160
51 V(I) = V(I)/UINF SPEC2170
D0114I =1,NSP SPEC2180
D0114J =1,NP SPEC2190
114 SY(I,J) = Y(I,J) SPEC2200
D0115I =1,NSP SPEC2210
D0115J =1,NP SPEC2220
115 Y(ISN(I),J) = SY(I,J) SPEC2230
RETURN SPEC2240
END SPEC2250
SUBROUTINE SOLVE (ZO, Z1)
C-----THIS SUBROUTINE SOLVES THE DIFFERENTIAL EQUATION
C
C     A(X)Z'' + B(X)Z' + C(X)Z = D(X)
C
C     WITH BOUNDARY CONDITIONS Z(0) = Z0, AND Z(1) = Z1. THE NUMERICAL
C
C     INTEGRATION IS PERFORMED WITH NETA POINTS IN THE DOMAIN OF
C
C     INTEREST. THE VARIABLE COEFFICIENTS A, B, C, AND D MUST BE
C
C     EVALUATED AT NETA2=NETA-2 INTERIOR POINTS AND STORED IN SUB.
C
C     DIAG, SUP, AND B, RESPECTIVELY. THE SOLUTION IS RETURNED IN B.
C
COMMON /NETI/NETA1, NETA2
COMMON /VECTOR/SUB(60), DIAG(60), SUP(60), B(60)
COMMON /YL/ETA(60), YOND(60)
DX I = ETA(I + 2) - ETA(I)
DO40J = 2, NETA1
DX = ETA(J + 1) - ETA(J)
J1 = J - 1
J2 = J - 2

CA = SUB(J1)*C6(DX, DX1) + DIAG(J1)*C3(DX, DX1)
CB = SUB(J1)*C5(DX, DX1) + DIAG(J1)*C2(DX, DX1) + SUP(J1)
CC = SUB(J1)*C4(DX, DX1) + DIAG(J1)*C1(DX, DX1)

DIAG(J1) = CB
SUP(J1) = CC
IF(J1.EQ.1) GO TO 20
SUBL(J2) = CA
GO TO 40

20 BC = CA

40 DX1 = DX
B(1) = B(1) - BC*ZO
B(NETA2) = B(NETA2) - SUP(NETA2)*Z1
CALL TRID (NETA2)
RETURN
END
SUBROUTINE CHEMEQ(NI,NF)CHEM 10
C************************CHEM 20
C THIS SUBPROGRAM IS A REVISION OF A PROGRAM ORIGINALLY REPORTED CHEM 30
C PRESSURE ARRAY,PP(N), TEMPERATURE ARRAY, TT(N), AND AN ARRAY CHEM 50
C OF ELEMENTAL MASS FRACTIONS-CC(I,N), THE EQUILIBRIUM SPECIES CHEM 60
C MASS FRACTIONS AT EACH POINT N REPRESENTED BY THE GIVEN ARRAYS. CHEM 70
C THE EQUILIBRIUM COMPOSITIONS ARE STORED IN THE MATRIX CE(I,N). CHEM 80
C
DONALD D. ESCHCHEM 100
LOUISIANA STATE UNIVERSITYCHEM 110
AUGUST 7, 1970CHEM 120

C IN = INITIAL POINT FOR EQUILIBRIUM CALCULATIONS.CHEM 130
C NF = FINAL POINTCHEM 140
C
COMMON/WALL/RW,PRM,TWOLD,FLUX(20),CWALL(20),ECWALL(5)CHEM 150
COMMON/SS,TOL,NDBLGCHEM 160
COMMON/EQ1/AI(20),RI(20),CI(20),DI(20),EI(20),FI(20),GI(20)CHEM 170
COMMON/EQ2/AA(20*5),ICODE(20)CHEM 180
COMMON/THERM1/C(20),FORT(20)CHEM 190
COMMON/ID/SP(20),EL(5)CHEM 200
COMMON/NUMBER/NS,NNS,MM,NCCHEM 210
COMMON/WT/XM(20),AWT(5)CHEM 220
COMMON/RH/DUD,DPHI,TD,RZB,PD,HD,HTOTALCHEM 230
COMMON/DY/DYDT(20,60)CHEM 240
COMMON/PROP1/PP(60),RO(60),TT(60),AMW(60),CE(20,60),CC(5,60)CHEM 250
DIMENSION R(7,7),B(7,1),YINT(20),FY(20),PI(7),FSUM(20),YSUM(20)CHEM 260
1,X(20),DELT(20),XLAM(20)CHEM 270
DIMENSION E(5),AB(5),Y(20)CHEM 280
DIMENSION EOLD(5)CHEM 290

CHEM 300
CHEM 310
CHEM 320
CHEM 330
CHEM 340
CHEM 350
5 CONTINUE

C MA=1

C------INITIAL GUESS FOR EQUILIBRIUM CALCULATIONS....

C DO10 I=1,NS

10 Y(I) = CWALL(I)*AMW(NI)/XMW(I)

C------COMPUTE THE SIZE OF THE MATRIX

C NA=MM+1

C NS=NUMBER OF SPECIES....

C CRIT=CRITERIA FOR CONVERGENCE.

C CRIT =TOL
XBETA=CRIT
BETA=0.
LL=NS+1
TOLD=0.0

C THE REMAINDER OF THE PROGRAM COMPUTES EQUILIBRIUM COMPOSITIONS
C CORRESPONDING TO THE ELEMENTAL MASS FRACTIONS IN THE CC-ARRAY
C FROM POINT N = NI TO POINT N = NF.

C SUM = 0.
D01511 I=1,MM

1511 SUM = SUM + CC(I,1)
D02011 I=1,MM

2011 EOLD(I) = CC(I,1)/SUM
D05000 N=NI,NF
T = T(T(N)*TD
P=PP(N)
BETOLD=0.0
SUM=0.0
DO 15 I=1,MM
  SUM=SUM + CC(I,N)
DO 20 I=1,MM
  IF(CC(I,N)*LT.1.0E-10) CC(I,N)=1.0E-10
20  E(I)=CC(I,N)/SUM

C
  CALL ALTERY(E,EOLD,Y,TOLD)
C
  TINCR=ABS(T-TOLD)
  IF(TINCR.LE.0.01)GOTO1750

22  NT=1
DO 25 J=1,MM
  BB(J)=0.0
DO 25 I=1,NS
  BB(J)=BB(J)+AA(I,J)*Y(I)

C
  CALL THERMO(T,P)
C
  C----THERMO SUBPROGRAM CALCULATES F/RT FOR EACH COMPONENT
C
  C----SET-UP THE R-MATRIX AND THE B-VECTOR
C
40  YBAR=0.0
   DO50 I=1,NS
50  YBAR=YBAR+Y(I)

C
  YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES
C
C----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES
C
DO60 I=1,NS
FAC = Y(I)/YBAR

IF (FAC .LT. 1.0E-73) FAC = 1.0E-73

60 FY(I) = Y(I)*(C(I) + ALOG(FAC))

C

C----- PROCEED TO CONSTRUCT THE R MATRIX
C

C----- INITIALIZE TO ZERO
C

DO 75 J=1,NA
    DO 75 K=1,NA
    R(J,K) = 0.0

75

DO 90 J=1,MM
    DO 90 K=J,MM
    SUM = 0.
    DO 90 I = 1,NS
    SUM = SUM + AA(I,J)*AA(I,K)*Y(I)
    R(J,K) = SUM
    R(K,J) = SUM

90

DO 103 K=1,MM
    SUM = 0.
    DO 101 I=1,NS
    SUM = SUM + AA(I,K)*Y(I)
    R(K,NA) = SUM
    R(NA,K) = SUM

101

103 CONTINUE

C

C----- PROCEED TO CALCULATE THE VECTOR B
C

DO 140 J=1,MM
    SUM = 0.
    DO 130 I = 1,NS
    SUM = SUM + AA(I,J)*FY(I)
130

140 B(J,1) = SUM + BB(J)
SUM=0
DO 150 I=1,NS
150 SUM=SUM+FY(I)
B(NA,I)=SUM

C-----MATRIX INVERSION IS CALLED TO PROVIDE THE SOLUTION FOR
C THE LINEARIZED EQUATIONS. THE SOLUTION OF THE EQUATIONS
C GIVES THE LAGRANGIAN MULTIPLIERS NEEDED TO COMPUTE THE MOLES
C OF EACH GAS SPECIES.
C
CALL MATINV(R,NA,B,NA,NMAX)
156 CONTINUE
C
DO 160 I=1,NA
C
PI(I)=LAGRANGIAN MULTIPLIERS
C
160 PI(I)=B(I,1)
U=PI(NA)
XBAR=U*YBAR
C
C-----COMPUTE THE MOLES OF EACH SPECIE.....
C
DO 170 I=1,NS
170 FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR
DO 200 I=1,NS
PSUM=0
DO 180 J=1,MM
180 PSUM=PSUM+PI(J)*AA(I,J)
YSUM(I)=PSUM*Y(I)
200 X(I)=FSUM(I)+YSUM(I)
C
C-----CHECK IF CONVERGENCE CRITERIA HAS BEEN MET. IF SO, GO TO 800
C
BETA=0.0
DO215 I=1,NS
DELT(I)=X(I)-Y(I)
215 BETA=BETA+ABS(DELT(I))
IF(BETA.GTBETOLD)GOT0216
IF(BETA.LT.XBETA)GOT0800
216 CONTINUE
C
C------COMPLETE THE CONVERGENCE PARAMETER XLAMBD
C
XLAMBD=1.0
DO210 I=1,NS
IF(ABS(DELT(I)).LT.1.0E-20)DELT(I)=0.0
IF(DELT(I).GE.0.0)GOT0210
IF(X(I).GE.0.0)GOT0210
XLAM(I)=-Y(I)/DELT(I)
XLAMBD=AMIN1(XLAMBD,XLAM(I))
XLAMBD=.99*XLAMBD
210 CONTINUE
XLAM1=XLAMBD
IF(XLAM1.EQ.0.0)XLAM1=1.0E-5
DEBAR=0.0
DO220 I=1,NS
220 DEBAR=DEBAR+DELT(I)
C
C------DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.
C
C APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE
C NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE
C VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF
C Y(I) AS WAS USED IN THE PREVIOUS ITERATION
C
C------DETERMINE THE FREE ENERGY GRADIENT. IF POSITIVE REDUCE XLAMDBA
C
C DFDL=FREE ENERGY GRADIENT
C
DFDL = 0

DO 280 I = 1, NS
FAC = (Y(I) + XLAMBD * DELT(I)) / (YBAR + XLAMBD * DEBAR)
   IF (FAC .LT. 1.E-73) FAC = 1.E-73
   C260 DERF = (DELT(I) * YBAR - DEBAR * Y(I)) / (YBAR + XLAMBD * DEBAR)
   C280 DFDL = DFDL + (C(I) - ALOG(FAC)) + DERF
   280 DFDL = DFDL + DELT(I) * (C(I) + ALOG(FAC))
   IF (DFDL .LT. 0.000) GOTO 300
   XLAMBD = 8 * XLAMBD
   IF (XLAMBD .GT. 1.E-6) GOTO 230
   CHEM2110
   CHEM2120
   CHEM2130
   CHEM2140
   CHEM2150
   CHEM2160
   CHEM2170
   CHEM2180
   CHEM2190
   CHEM2200
   CHEM2210
   CHEM2220
   CHEM2230
   CHEM2240
   CHEM2250
   CHEM2260
   CHEM2270
   CHEM2280
   CHEM2290
   CHEM2300
   CHEM2310
   CHEM2320
   CHEM2330
   CHEM2340
   CHEM2350
   CHEM2360
   CHEM2370
   CHEM2380
   CHEM2390
   CHEM2400
   CHEM2410
   CHEM2420
   CHEM2430
   CHEM2440
   CHEM2450

C THE VALUE OF XLAMBD THAT ASSURES CONVERGENCE HAS BEEN FOUND
C
DO 350 I = 1, NS
   IF (XLAMBD .GT. 1.E-6) GOTO 330
   IF (DFDL .LT. 0.000) GOTO 300
   XLAMBD = XAMBD + 1.E-6
   CHEM2300
   CHEM2310
   CHEM2320
   CHEM2330
   CHEM2340
   CHEM2350
   CHEM2360
   CHEM2370
   CHEM2380
   CHEM2390
   CHEM2400
   CHEM2410
   CHEM2420
   CHEM2430
   CHEM2440
   CHEM2450

C CALCULATE THE NEW COMPOSITION FOR THE NEXT ITERATION
C
Y(I) = Y(I) + XLAMBD * DELT(I) * 1
GOTO 340

330 Y(I) = Y(I) + XLAMBD * DELT(I)
340 IF (Y(I) .LT. 0.) Y(I) = 1.E-73
350 CONTINUE

C NT = NT + 1
BETOLD = BETA
TOLD = T

C IF THE NUMBER OF ITERATIONS EXCEED 900 STOP COMPUTATIONS
C
IF (NT .GT. 900) GOTO 6000
GOTO 40

800 CONTINUE
CONVERT EQUILIBRIUM MOLE FRACTIONS TO MASS FRACTIONS AND STORE THESE VALUES IN THE CE-MATRIX. AMW(N) IS THE AVERAGE MOLECULAR WEIGHT AT THE POINT. N.

SUMY=0.0
DO900 I=1,NS
900 SUMY=SUMY+Y(I)
AMW(N) = 0.0
DO1000 I=1,NS
Y(I)=Y(I)/SUMY
1000 AMW(N) = AMW(N) + Y(I)*XMW(I)
DO1005 I=1,NS
1005 CE(I,N) = Y(I)*XMW(I)/AMW(N)
GOTO1800

IF THE TEMPERATURE CHANGE IS LESS THAN 50 DEGREES FROM LAST F. E. M. CALCULATION ASSUME CURRENT VALUES AS EQUAL TO LAST VALUES.

DO1760 I=1,NS
1760 CE(I,N)=CE(I,N-1)
AMW(N)=AMW(N-1)
1800 CONTINUE

OPTIONAL OUTPUT OF POSITION * TEMPERATURE AND EQUILIBRIUM COMPOSITIONS.

IF(NDBUG.LT.1)GOTO3000
PRINT 2000,P,T,*,NT
2000 FORMAT(/,' T(0K) = ''F5.3'','F6.0','S5X','NUMBER OF ITERATIONS ''F5.3'','S5X','C(I,N)''),/)
PRINT 2005,(SP(I),Y(I),CE(I,N),I=1,NS)
2005 FORMAT(1X,A4,2E18.8)
C
3000 CONTINUE
3300 XBETA=CRIT
5000 CONTINUE
8000 CONTINUE
   RETURN
6000 PRINT6001
6001 FORMAT(' NUMBER OF ITERATIONS EXCEEDED 900, PROGRAM TERMINATING')
   RETURN
   END
SUBROUTINE ALTERY(E,EOLD,Y,TOLD)
COMMON/WT/SMW(20),AWT(5)
COMMON/NUMBER/NSP,NNS,NE,NC
COMMON/EQ2/AA(20,5),ICODE(20)
COMMON/ELSP/LSP(5)
COMMON/SS,TOL,NDBUG
DIMENSION E(5),Y(20),B(5),EOLD(5)
C
IF(NDBUG GT 1)PRINT101
101 FORMAT(' INITIAL GUESS ON MOLE FRACTIONS UPDATED')
C
C----ASSUME ALL SPECIES HAVE THE SAME COMPOSITION.......
C
C
C----COMPUTE GRAM-ATOMS OF EACH ELEMENT FROM KNOWN ELEMENTAL COMPOSITION AND THE MAXIMUM POSSIBLE MOLECULAR WEIGHT.......
C
C
DO20 J=1,NE
IF(E(J)*GTE OE-8)GOTO20
DO15 I=1,NSP
IF(AA(I,J)*LEOE)GOTO15
Y(I)=OE-12
15 CONTINUE
20 E(J)=E(J)*100/AWT(J)
C
C----CALCULATE FOR EACH ELEMENT, THE NUMBER OF G-ATOMS BASED ON THE FIRST GUESS. ADJUST THE COMPOSITION OF EACH ELEMENT-SPECIE AS REQUIRED.......
C
C
DO30 J=1,NE
R(J)=0.0
DO30 I=1,NSP
30 B(J)=B(J)+AA(I,J)*Y(I)
DO40 J=1,NE
EOLD(J) = E(J)
40  \[ Y(\text{LSP}(J)) = Y(\text{LSP}(J)) + (E(J) - B(J)) \]
TOLD = 0.0
RETURN
END
SUBROUTINE THERMO(T,P)

C
C

THER 10
THER 20
THER 30
C------SUBROUTINE THERMO CALCULATES THE FREE ENERGY FUNCTION FOR EACH CHEMICAL SPECIE.

COMMON/NUMBER/NQ,NNS,NE,NC
COMMON/EQI/AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20),THER40
COMMON/EQ2/AA(20),ICODE(20)
COMMON/Therm1/C(20),FORT(20)

T=TEMPERATURE IN OK

Ti=T
T2=Ti*T
T3=T2*T
T4=T3*T
T5=T4*T

THER 40

C------CALCULATE THE FREE ENERGY FUNCTION FCRT(I)

FORT(I)=FREE ENERGY FUNCTION

DO 41 I=1,NQ
IF(T*GT.6000.)GOT06205
FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.
   -FI(I)*T4/20.+FI(I)/T-GI(I)
   IF(ICODE(I).EQ.1)GOT041
   C(I)=FORT(I)+ALOG(P)
   GOT041
6205 FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.
   -EI(I)*T4/20.+FII(I)/T-GII(I)
   IF(ICODE(I).EQ.1)GOT041
   C(I)=FORT(I)+ALOG(P)
   41 CONTINUE

THER 50
THER 60
THER 70
THER 80
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THER 360
THER 370
THER 380
SUBROUTINE MATINV(A,N,B,M,NMAX)

MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS

DIMENSION A(7,7), B(7,1), IPIVOT(7), INDEX(7,2)

EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUMN), (AMAX,T,SWAP)

INITIALIZATION

5 ISCALE=0
6 R1=10.0*18
7 R2=1.0/R1
10 DETERM=1.0
15 DO 20 J=1,N
20 IPIVOT(J)=
30 DO 550 I=1,N

SEARCH FOR PIVOT ELEMENT

40 AMAX=0.0
45 DO 105 J=1,N
50 IF (IPIVOT(J)-1)60,10105
60 DO 100 K=1,N
70 IF (IPIVOT(K)-1)80,10100
80 IF (ABS(AMAX)=ABS(A(J,K)))85,100,100
85 IROW=J
90 ICOLUM=K
95 AMAX=A(J,K)
100 CONTINUE
101 CONTINUE
IF (AMAX)110,110
106 DETERM=0.0
ISCALE=0
GO TO 740
110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
C INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL

130 IF (IROW-ICOLUM)140.260.140
140 DETERM=-DETERM
150 DO 200 L=1,N
160 SWAP=A(IROW,L)
170 A(IROW,L)=A(ICOLUM,L)
200 A(ICOLUM,L)=SWAP
205 IF(M)260.260.210
210 DO 250 L=1,M
220 SWAP=B(IROW,L)
230 B(IROW,L)=B(ICOLUM,L)
250 B(ICOLUM,L)=SWAP
260 INDEX(I,1)=IROW
270 INDEX(I,2)=ICOLUM
310 PIVOT=A(ICOLUM,ICOLUM)

C SCALE THE DETERMINANT

1000 PIVOT=PIVOT
1005 IF(ABS(DETERM)-R1)1030.1010.1010
1010 DETERM=DETERM/R1
   ISCALE=ISCALE+1
   IF(ABS(DETERM)-R1)1060.1020.1020
1020 DETERM=DETERM/R1
   ISCALE=ISCALE+1
   GO TO 1060
1030 IF(ABS(DETERM)-R2)1040.1040.1060
1040 DETERM=DETERM*R1
   ISCALE=ISCALE-1
   IF(ABS(DETERM)-R2)1050.1050.1060
1050 DETERM=DETERM*R1
   ISCALE=ISCALE-1
1060 IF(ABS(PIVOT)-R1)1090.1070.1070
1070 PIVOTI=PIVOTI/R1
  ISCALE=ISCALE+1
  IF(ABS(PIVOTI)-R1)320,1080,1080
1080 PIVOTI=PIVOTI/R1
  ISCALE=ISCALE+1
  GO TO 320
1090 IF(ABS(PIVOTI)-R2)2000,2000,320
2000 PIVOTI=PIVOTI*R1
  ISCALE=ISCALE-1
  IF(ABS(PIVOTI)-R2)2010,2010,320
2010 PIVOTI=PIVOTI*R1
  ISCALE=ISCALE-1
320 DETERM=DETERM*PIVOTI

C
C   DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
330 A(ICOLUML,ICOLUML)=1.0
340 DO 350 L=1,N
350 A(ICOLUML,L)=A(ICOLUML,L)/PIVOT
355 IF(M) 380,380,360
360 DO 370 L=1,M
370 B(ICOLUML,L)=B(ICOLUML,L)/PIVOT

C
C   REDUCE NON-PIVCT RCWS
C
380 DO 550 L1=1,N
390 IF(L1-ICOLUML)400,550,400
400 T=A(L1,ICOLUML)
410 A(L1,ICOLUML)=0.0
420 A(L1,ICOLUML)=A(L1,ICOLUML)-A(ICOLUML,L)*T
430 DO 450 L=1,N
440 A(L1,L)=A(L1,L)-A(ICOLUML,L)*T
455 IF(M) 550,550,460
460 DO 500 L=1,M
500 B(L1,L)=B(L1,L)-B(ICOLUML,L)*T
550 CONTINUE
C   INTERCHANGE COLUMNS

   600 DO 710 I=1,N

C

   610 L=N+1-I
   620 IF(INDEX(L,1)-INDEX(L,2))630,710,630
   630 JROW=INDEX(L,1)
   640 JCOLUM=INDEX(L,2)
   650 DO 705 K=1,N
   660 SWAP=A(K,JROW)
   670 A(K,JROW)=A(K,JCOLUM)
   680 A(K,JCOLUM)=SWAP
   705 CONTINUE

710 CONTINUE

740 RETURN

   END
SUBROUTINE PROPRT(NSP,NI,NF)  

C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *

C SUBROUTINE FOR THE CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES

C

C NOMENCLATURE

C Y(I).....MOLE FRACTION OF COMPONENT I
C C(I,N)....MASS FRACTION OF COMPONENT I AT POINT N
C T(I).....TEMPERATURE, DEG. K
C CP(I).....SPECIES SPECIFIC HEAT, CAL/GMOLE OF I-K
C CPM(N)....MIXTURE SPECIFIC HEAT, CAL/GMOLE OF M-K
C H(I).....SPECIES ENTHALPY, CAL/GMOLE OF I
C HM(N).....MIXTURE ENTHALPY, CAL/GMOLE OF M
C VIS(I)....SPECIES VISCOSITY, LBM/FT-SEC
C VISM(N)....MIXTURE VISCOSITY, LBM/FT-SEC
C TC(I).....SPECIES THERMAL CONDUCTIVITY, BTU/FT-SEC-DEG. R
C TCM(N)....MIXTURE THERMAL CONDUCTIVITY, BTU/FT-SEC-DEG. R

COMMON /BLOCK1/VI(20),V2(20),V3(20)
COMMON/BLOCK3/K1(20),K2(20)
COMMON/FOI/AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20)

DIMENSION PHI(20,20),YPHI(20),Y(20),TC(20),VIS(20)
DIMENSION SAMW(2)
REAL MUMUDZK,K2
DATA R /1.98716/
DOSOON=NI,NF
T1 = T(N) * TD
T2 = T1 * T1
T3 = T2 * T1
T4 = T3 * T1
T5 = T4 * T1
DO150 I = 1, NSP
  IF(TI ≥ GT * 6000) G0TC 50
  CP(I, N) = (AI(I) + BI(I) * T1 + CI(I) * T2 + DI(I) * T3 + EI(I) * T4) * R
  H(I, N) = (AI(I) * T1 + BI(I) * T2 / 2 + CI(I) * T3 / 3 + DI(I) * T4 / 4 + EI(I) * T5 / 5 + FI(I)) * R
GOTO 100
DO 50 CP(I, N) = (AI(I) + BI(I) * T1 + CI(I) * T2 + DI(I) * T3 + EI(I) * T4) * R
H(I, N) = (AI(I) * T1 + BI(I) * T2 / 2 + CI(I) * T3 / 3 + DI(I) * T4 / 4 + EI(I) * T5 / 5 + FI(I)) * R
DO 150 I = 1, NSP
  X = EI(I) * T5 / 5 + FI(I)) * R
100 Y(I) = C(I, N) * AMW(N) / SMW(I)
  VIS(I) = (V1(I) + V2(I) + V3(I) + T2) * 1.0E-05
  TC(I) = (K1(I) + K2(I) * T1) * 1.0E-5
150 CONTINUE

C------CALCULATE PHI(I, J) PARAMETERS FOR MIXTURE PROPERTIES

C DO 200 I = 1, NSP
   VIS12 = SQRT(VIS(I) / VIS(J))
   SMW14 = SMW(J) / SMW(I) * 0.25
   PHI(I, J) = 3.54 * ((1 + VIS12 * SMW14) ** 2) / SQRT(1 + SMW(I) / SMW(J))
200 CONTINUE

C------CALCULATION OF MIXTURE PROPERTIES

C DO 250 I = 1, NSP
   YPHI(I) = 0.0
   YPHI(I) = YPHI(I) + Y(J) * PHI(I, J)
250 CONTINUE

VISM(N) = 0.0
TCM(N) = 0.0
DO 300 I=1,NSP
   IF(Y(I)*LT*1.E-5) GO TO 300
   VISM(N)=VISM(N)+Y(I)*VIS(I)/YPHI(I)
300 TCM(N) = TCM(N) + Y(I)*TC(I)/YPHI(I)
500 CONTINUE
C
C----- NONDIMENSIONALIZE QUANTITIES -----C
DO 550 N=NI,NF
   VISM(N) = VISM(N)/MUDZ
   TCM(N) = TCM(N)*AKNF
   RM(I)=RHO(N)*VISM(N)
   CPM(N) = 0.
   HM(N) = 0.
DO 550 I=1,NSP
   CP(I,N) = CP(I,N)*CPNF/MW(I)
   H(I,N) = H(I,N)*HNF*1.80/MW(I)
   CPM(N) = CPM(N) + CP(I,N)*C(I,N)
   HM(N) = HM(N) + H(I,N)*C(I,N)
550 CONTINUE
RETURN
END
SUBROUTINE STPSZE

*** ROUTINE TO ADJUST STEP SIZE AS NEEDED ***

TO MAINTAIN ACCURACY ***

COMMON /DEL/ DELTA, DTIL, DTILS
COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LXI, ITM, IEM, NETA
COMMON/PROP1/PI(60), RHO(60), G(60), AMW(60), C(20*60), EC(5,60)
COMMON/PROP2/ MU(60), RM(60), AK(60)
COMMON/PROP3/CPS(20*60), HS(20*60), CP(60), HM(60)
COMMON /RH/ DUD, DPHI, TD, RZE, PD, HD, HTOTAL
COMMON /RFLUX/ E(60), IRAD, ITYPE
COMMON /VEL/ F(60), FC(60), Z(60), V(60)
COMMON/WALL/ RW, PW, TWOLD, FLUX(20), CWALL(20), ECWALL(5)
COMMON /YL/ ETA(60), YOLD(60)
COMMON /OLD/ TOLD(60), EOLD(60), RHOS(60)

N=2
1 CONTINUE
   12=2
   IF (NETA.GE. 59) GO TO 5
2 CONTINUE
   DO 2 I=N*NETA
   L=I
   CHECK = ABS(G(I)-G(I-1))
   IF (CHECK .GT. 0.05) GO TO 3
   CONTINUE
   GO TO 5
3 CONTINUE
   M = NETA - L + 1
   DO 4 I=1,M
$K = \text{NETA} - 1 + 1$

$G(K+1) = G(K)$

$F(K+1) = F(K)$

$\text{DO 100 JJ}=1,5$

$100 \quad EC(JJ,K+1) = EC(JJ,K)$

$\text{TOLD}(K+1) = \text{TOLD}(K)$

$\text{RHOS}(K+1) = \text{RHOS}(K)$

$\text{RHO}(K+1) = \text{RHO}(K)$

$\text{RM}(K+1) = \text{RM}(K)$

$\text{IF}(\text{IRAD}=3) \quad E(K+1) = E(K)$

$\text{ETA}(K+1) = \text{ETA}(K)$

$\text{CONTINUE}$

$C$

$G(L) = (G(L-1) + G(L+1)) / 2.0$

$F(L) = (F(L-1) + F(L+1)) / 2.0$

$\text{DO 101 JJ}=1,5$

$101 \quad EC(JJ,L) = (EC(JJ,L-1) + EC(JJ,L+1)) / 2.0$

$\text{TOLD}(L) = (\text{TOLD}(L-1) + \text{TOLD}(L+1)) / 2.0$

$\text{RHOS}(L) = (\text{RHOS}(L-1) + \text{RHOS}(L+1)) / 2.0$

$\text{RHO}(L) = (\text{RHO}(L-1) + \text{RHO}(L+1)) / 2.0$

$\text{RM}(L) = (\text{RM}(L-1) + \text{RM}(L+1)) / 2.0$

$\text{IF}(\text{IRAD}=3) \quad E(L) = (E(L-1) + E(L+1)) / 2.0$

$\text{ETA}(L) = (\text{ETA}(L-1) + \text{ETA}(L+1)) / 2.0$

$\text{NETA} = \text{NETA} + 1$

$N = L$

$C$

$\text{IF}(\text{NETA} \lt 59) \text{ GO TO 1}$

$C$

$5 \text{ CONTINUE}$

$C$

$\text{IF}(I2 \geq \text{NETA}) \text{ GC TO 10}$

$\text{DO 6 } I = I2, \text{NETA}, 2$

$L = I$

$\text{IF}(L \leq \text{NETA}) \text{ GO TO 6}$

$\text{IF}(\text{ETA}(I) \leq 0.98) \text{ GO TO 6}$
CHECK =ABS(G(I+1) - G(I-1))
IF(CHECK .LT. 0.005) GO TO 7
   CONTINUE
C
GO TO 10
7 CONTINUE
I2=L+1
IF(ETA(L+1)-ETA(L-1) .GT. .04) GO TO 5
C
DO 8 I=L,NETA
   G(I) = G(I+1)
   F(I) = F(I+1)
   DO102 J=1,5
102 EC(JJ,I)=EC(JJ,I+1)
   TOLD(I)=TOLD(I+1)
   RHOS(I)=RHOS(I+1)
   RHO(I) = RHO(I+1)
   RM (I) = RM (I+1)
   IF(IRAD.EQ.3) E(I) =E(I+1)
   ETA(I)=ETA(I+1)
8 CONTINUE
C
NETA=NETA-1
IF (NETA .GT. 1) GO TO 5
C
10 CONTINUE
NN = NETA-2
DO 20 I=1,NN
   Z(I) = ETA(I+1)/DTIL
20 CONTINUE
RETURN
END
SUBROUTINE TRID (M)
C***** TRID -- TRIDIAGONAL EQUATION SOLVER OBTAINED FROM CONTE P-184 *** TRID
C SUBROUTINE SOLVES AX = B FOR THE VECTOR X WHERE A IS TRIDIAGONAL TRID
C M = ORDER OF SYSTEM TRID
C SUP = SUPER DIAGONAL OF A TRID
C SUB = SUB DIAGONAL OF A TRID
C DIAG = MAIN DIAGONAL OF A TRID
C B = CONSTANT VECTOR TRID
C SUP AND DIAG ARE DESTROYED TRID
C SOLUTION VECTOR IS RETURNED IN B TRID
C
COMMON/VECTOR/ SUB(60), DIAG(60), SUP(60), B(60)
C
N = M TRID
NN = N - 1 TRID
SUP(1) = SUP(1)/DIAG(1) TRID
B(1) = B(1)/DIAG(1) TRID
DO 10 I=2,N TRID
II = I - 1 TRID
C----- DECOMPOSE A TO FORM A = LU WHERE L IS LOWER TRIANGULAR, AND U IS UPPER TRIANGULAR ------
C DIAG(I) = DIAG(I) - SUP(II)*SUB(II) TRID
IF(I .EQ. N) GO TO 10 TRID
SUP(II) = SUP(II) / DIAG(I) TRID
C----- COMPUTE Z WHERE LZ = B TRID
10 B(I) = (B(I) - SUB(II) * B(II))/ DIAG(I) TRID
C----- COMPUTE X BY BACK SUBSTITUTION WHERE UX = Z TRID
DO 20 K =1,NN TRID
I = N - K TRID
20 B(I) = B(I) - SUP(I) * B(I+1) TRID
RETURN TRID
END
FUNCTION QUAD (X, FX, I)

** TRAPEZOIDAL QUADRATURE FUNCTION **

DIMENSION X(60), FX(60)
DX = X(I) - X(I-1)
QUAD = (DX/2.0) * (FX(I) + FX(I-1))
RETURN
END
SUBROUTINE EFLUX

COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LXI, ITM, IEM, NETA
COMMON /RH/ DUD, DPHI, TD, RZB, PD, HD, HTOTAL
COMMON /RFUX/ E(60), IRAD, ITYPE
COMMON /PROPI/ PI(60), RHO(60), T(60), AMW(60), C(20,60), CC(5,60)
DIMENSION EOLD(60)

DO 100 I=1,NETA
  IF(IEM.GT.1) EOLD(I) = E(I)

PL = ALOG10(PI(I))
TSI = T(I)*TD
TS = 1100.0*PL + 13800.
IF (TS - TSI ) 300.260.200
  200 FP = 10.**((.0005 *TSI + 1.15*PL - 3.15)
    GO TO 350
  300 EP = 10.**((1.875 *PL + 3.903
C **** EP HAS UNITS OF WATTS/CM**3 ***
C 350 E(I) = (EP*R/( RINF *UINF2 *U INF)) * 20866.0
C 400 E(I) = E(I) *RZB
C IF(IEM.GT.1) E(I) = .6 *E(I) +.4 *EOLD(I)
C **** E IS NONDIMENSIONAL ***
C 100 CONTINUE
RETURN
END
FUNCTION C1 (DX,DX1)
C1 = DX1/(DX/(DX+DX1))
RETURN
END
FUNCTION C2 (DX-DX1)
C2 = (DX-DX1)/DX/DX1
RETURN
END
FUNCTION C3 (DX+DX1)
C3 = -DX/DX1/(DX+DX1)
RETURN
END
FUNCTION C4 (DX, DX1)
C4 = 2 * D0 / DX / (DX + DX1)
RETURN
END
FUNCTION C5 (DX, DX1)
C5 = -2 * D0 / DX / DX1
RETURN
END
FUNCTION C6 (DX, DX1)
C6 = 2.0 * D0 / DX1 / (DX + DX1)
RETURN
END
BLOCK DATA
COMMON/FINV/NHVL,NIHVC,FHVC(12),DJ(9),HVJ(9),ZKZ DATA 10
COMMON/FRSTRM/U INF, R INF, UINF2, R, RE, LX1, ITM, IEM, NETA DATA 20
COMMON/GUESS/TG1(60),TG2(60) DATA 30
COMMON/PROP1/PI(60),RHO(60),T(60),AMW(60),C(20,60),EC(5,60) DATA 40
COMMON/PROP2/MU(60),RM(60),AK(60) DATA 50
COMMON/PROP3/CPS(20,60),HS(20,60),CP(60),HM(60) DATA 60
COMMON/NUMBER/NSP.*NS,NE,NC DATA 70
COMMON/ELSP/LSP(5) DATA 80
COMMON/ID/SP(20),EL(5) DATA 90
COMMON/WT/SMW(20),AWT(5) DATA 100
COMMON/BLOCK1/V1(20),V2(20),V3(20) DATA 110
COMMON/BLOCK3/K1(20),K2(20) DATA 120
COMMON/EQ1/AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20) DATA 130
X
AII(20),AII(20),AII(20),DI(20),EI(20),FI(20),GI(20) DATA 140
COMMON/EQ2/AA(20,5),ICODE(20) DATA 150
COMMON/EQ3/IA(20,5) DATA 160
REAL K1,K2 DATA 170
COMMON/CK/ISN(20),MWT(19) DATA 180
REAL MWT DATA 190
DATA ISN/
1 11, 8, 19, 12, 20, 14, 13, 18, 10, 9, 2, 4, 6, DATA 200
2 3, 5, 7, 15, 16, 17, 1/ DATA 210
DATA MWT/
2 02,016, 01.008, 28.016, 14.008, 14.008, 16.000, 16.000, DATA 230
3 26.038, 37.041, 49.052/ DATA 240
DATA NETA/0/ DATA 250
DATA RHO /25.1,14.3,8,85.6,50,4.37,3.01,2.49,2.17,1.90,1.67,1.46, DATA 260
1 1.29,1.16,1.08,1.03,1.00,1.04*1.0/ DATA 270
DATA RM /10.0,7.7,7.5,8.9,5.10,4.18,3.54,3.13,1.10,2.83,2.48,2.09, DATA 280
1 1.72,1.42,1.22,1.09,1.02,4.4*1.0/ DATA 290
DATA TG1 /1.1033,1.2294,1.3531,1.4719,1.5777,1.6531,1.6867,1.7034,1.7145, DATA 300
1 1.7236,1.7321,1.7401,1.7479,1.7554,1.7628,1.7699,1.7759,1.7836,1.7902, DATA 310
2 1.7967,1.8030,1.8092,1.8153,1.8213,1.8272,1.8331,1.8389,1.8447,1.8504, DATA 320

| DATA AI/O | 0.3316E 01, 0.3221E 01, 0.2670E 01, 0.2474E 01, 0.2491E 01, 0.2727E 01, 0.2500E 01, 0.2612E 01, 0.2500E 01, 0.3358E 01 | DATA 710 |
| DATA 720 |
| DATA 730 |
| DATA 740 |
| DATA 750 |
| DATA 760 |
| DATA 770 |
| DATA 780 |
| DATA 790 |
| DATA 800 |
| DATA 810 |
| DATA 820 |
| DATA 830 |
| DATA 840 |
| DATA 850 |
| DATA 860 |
| DATA 870 |
| DATA 880 |
| DATA 890 |
| DATA 900 |
| DATA 910 |
| DATA 920 |
| DATA 930 |
| DATA 940 |
| DATA 950 |
| DATA 960 |
| DATA 970 |
| DATA 980 |
| DATA 990 |
| DATA 1000 |
| DATA 1010 |
| DATA 1020 |
| DATA 1030 |
| DATA 1040 |
| DATA 1050 |
SUBROUTINE LRAD

C ** THIS IS A DRIVER PROGRAM FOR SUBROUTINE TRANS WHICH CALCULATES **
C THE RADIATIVE FLUX DIVERGENCE THROUGH A ONE-DIMENSIONAL SLAB C
C FOR A GIVEN TEMPERATURE AND SPECIES DISTRIBUTION C

COMMON /SFLUX/QRI(3) LRAD 10
COMMON /TRN/NUT(60), FMC(12,60), FPC(12,60), LRAD 20
COMMON /TEST/ETZ(60), IEZ LRAD 30
COMMON /YL/ETA(60), YOND(60) LRAD 40
COMMON/PROP1/PI(60), RHC(60), T(60), AMW(60), C(20,60), EC(5,60) LRAD 50
COMMON/SIS/SY(20,60) LRAD 60
COMMON /FRSTM/U INF, RINF, UINF2, R, RE, LXI, ITM, IEM, NETA LRAD 70
COMMON /DEL/ DELTA, DTIL, DTILS LRAD 80
COMMON /NON/ROZ, MUCZ, RNDZ, AKNF, HNF, CFNF LRAD 90
COMMON /MAIN/KEEP, MAXE, MAXM, MAXD, IDG, MCONV, ECONV, DCONV, LT, IAB LRAD 100
COMMON /SIS/SI20(60) LRAD 110
COMMON /SPEC/MF, XMOL LRAD 120

DO100 CI=1,20
DO100 CJ=1,NETA
100 SY(I,J) = C(I,J)
DO200 CI=1,20
DO200 CJ=1,NETA
200 IF(C(I,J)*LT.0.)C(I,J) = 1.E-20

C ** NETA = NUMBER OF ETA POINTS C
C MF = 1 IF SPECIE MOLE FRACTIONS ARE INPUT AND NUMBER DENSITY C
C TO BE COMPUTED C
C 0 IF SPECIE NUMBER DENSITIES ARE INPUT LRAD 330
C NS = NUMBER OF SPECIES TO BE INPUT
C LINES=1 IF LINE CALCULATION IS TO BE DONE
C 0 IF ONLY CONTINUUM CALCULATION IS TO BE DONE
C IDG = 0 ONLY FINAL PRINT IS GIVEN
C 1 PRINT IS GIVEN FOR EACH ETA
C 99 COMPLETE PRINT

C ** R = BODY RADIUS (FT)
C DELTA = NONDIMENSIONAL STAND-OFF DISTANCE
C DTIL = TRANSFORMED STAND-OFF DISTANCE
C XMOL = 1.0 FOR RUN WITH MOLECULES
C 0.0 FOR RUN WITHOUT MOLECULES

C XMOL = 0.0
C XMOL= 1.0

C ** DETERMINE ETZ POINTS
C N2 = NETA-2
C K =0
C IEZ =0
C DO 20 I=1,N2+2
C K=K+1
C 20 ETZ(K) = ETA(I)
C ETZ(K+1) = ETA(NETA-1)
C ETZ(K+2) = ETA(NETA)
C IEZ = K +1

C ** COMPUTE THE Y COORDINATE **
C YOND(1) = 0.0
C SUM = 0.0
C DO 30 K=2,NETA
C DETA = ETA(K) -ETA(K-1)
C DETA = ETA(K) -ETA(K-1)
C SUM = SUM +DETA*(1./RHG(K) +1./RHO(K-1))/2.0
C YOND(K) = DTIL *SUM

LRAD 360
LRAD 370
LRAD 380
LRAD 390
LRAD 400
LRAD 410
LRAD 420
LRAD 430
LRAD 440
LRAD 450
LRAD 460
LRAD 470
LRAD 480
LRAD 490
LRAD 500
LRAD 510
LRAD 520
LRAD 530
LRAD 540
LRAD 550
LRAD 560
LRAD 570
LRAD 580
LRAD 590
LRAD 600
LRAD 610
LRAD 620
LRAD 630
LRAD 640
LRAD 650
LRAD 660
LRAD 670
LRAD 680
LRAD 690
LRAD 700
30 CONTINUE
DELTA = YOND(NETA)
DO 40 K=1,NETA
   YOND(K) = YOND(K)/YOND(NETA)
40 CONTINUE
C
LINES= 1
IDGS = IDG
IDG = 0
CALL TRANS(1)
IDG= IDGS
C ** INDEX IS NUMBER GIVEN SPECIE FOR USE IN STORING ARRAYS **
1 = O2
2 = N2
3 = O
4 = N
5 = E-
6 = C
7 = H
8 = C2
9 = H2
10 = CO
11 = C3
12 = C2H
DO300 I = 1,20
DO300 J=1,NETA
   C(I,J) = SY(I,J)
300 C(I,J) = SY(I,J)
RETURN
END
SUBROUTINE RADIN
COMMON /DBUG/ QLC(60), QCL(60), QLL(60), DQN(60), QCC(60),
1 BEEC(12,60), FMUC(12,60), EM(12,60),
2 EP(12,60), TAUC(12,60), BEEL(9,60),
3 QCCP(12), WMM(9,60), GMM(9,60),
4 EEM(9,60), XLMM(9,60), QLCP(9),
5 QCLP(9), QLLP(9), DELTA, IY, IYY,
6 WPP(9,60), GPP(9,60), EEP(9,60),
7 XLPP(9,60), FG(9,4), GP(9,4),
8 WN(9,4), FMUL(9,60), SSM(9,4,60),
9 GGM(9,4,60), ETAM(9,4,60), SBM(9,4,60),
A TAUL(9,60)

C ** GROUP 1 **
1 WN(1,1)=0.
2 FG(1,1)=\_.
3 GP(1,1)=0.
4 WN(1,2)=18.
5 WN(1,3)=15.
6 WN(1,4)=5.

C ** GROUP 2 **
1 WN(2,1)=3.0
2 WN(2,2)=5.0
3 WN(2,3)=11.0
4 WN(2,4)=10.

C ** GROUP 3 **
1 WN(3,1)=0.
2 FG(3,1)=\_.
3 GP(3,1)=0.
4 WN(3,2)=2.0
5 WN(3,3)=0.
6 FG(3,3)=\_.
7 GP(3,3)=0.
8 WN(3,4)=0.
9 FG(3,4)=\_.
A GP(3,4)=0.
C ** GROUP 4 **
WN(4,1) = 0
FG(4,1) = 0
GP(4,1) = 0
WN(4,2) = 8.0
WN(4,3) = 2.0
WN(4,4) = 0
FG(4,4) = 0
GP(4,4) = 0

C ** GROUP 5 **
WN(5,1) = 0
FG(5,1) = 0
GP(5,1) = 0
WN(5,2) = 14.0
WN(5,3) = 4.0
WN(5,4) = 1.0

C ** GROUP 6 **
WN(6,1) = 1.0
WN(6,2) = 4.0
WN(6,3) = 13.0
WN(6,4) = 2.0

C ** GROUP 7 **
WN(7,1) = 0
FG(7,1) = 0
GP(7,1) = 0
WN(7,2) = 6.0
WN(7,3) = 14.0
WN(7,4) = 3.0

C ** GROUP 8 **
WN(8,1) = 2.0
WN(8,2) = 2.0
WN(8,3) = 11.0
WN(8,4) = 15.0

C ** GROUP 9 **
WN(9,1) = 0

RADI 360
RADI 370
RADI 380
RADI 390
RADI 400
RADI 410
RADI 420
RADI 430
RADI 440
RADI 450
RADI 460
RADI 470
RADI 480
RADI 490
RADI 500
RADI 510
RADI 520
RADI 530
RADI 540
RADI 550
RADI 560
RADI 570
RADI 580
RADI 590
RADI 600
RADI 610
RADI 620
RADI 630
RADI 640
RADI 650
RADI 660
RADI 670
RADI 680
RADI 690
RADI 700
FG(9, 1) = 0.
GP(9, 1) = 0.
WN(9, 2) = 10.
WN(9, 3) = 11.
WN(9, 4) = 10.
RETURN
END
SUBROUTINE TRANS (ISU)
C
C-----THIS IS A MODIFIED VERSION OF SUBROUTINE TRANS FROM K WILSON
C TRANS IS DOCUMENTED IN LMSC-687209 APRIL 69
C
COMMON /ZPI/ ZPO(6), ZPN(6), ZPH(2), ZPC(7)
COMMON /FINV/ NHVL,NHVC,FHVVC(12), DJ(9), HVJ(9), ZKZ
COMMON /SFLUX/ QRI(3)
COMMON /TRN/ NUT(60), FMC(12,60), FPC(12,60),
1 FM(9,60), FP(9,60), LINES
COMMON /YL/ ETA(60), YD(60)
COMMON /PROP/ P (60), R(60), T(60), AYW(60), C (20,60), EC(5,60)
COMMON /FRSTRM/ U INF, RINF, UINF2, XL, RE, LXI, ITM, IEM, NES
COMMON /DEL/ W(1), DTIL, DTILS
COMMON /NON/RDZ, MDZ, AKN, HNF, CFNF
COMMON /MAIM/ KEEP, MAVE, MAXM, MAXD, IDG, MCONV, ECONV, DCONV, LT, IAB
COMMON /RFLUX/ E(60), IRAD, ITYPE
COMMON /RH/ DOD, DPHI, TD, RZB, PD, HD, HTOTAL
COMMON /WT/ SMW(20), AWT(5)
COMMON /TEST/ ETZ(60), IEZ
COMMON /NUMDEN/ SND02(60), SND2(60), SND(60), SNDN(60),
1 SNDE(60), SND(60),
2 SNDH(60), SNDH2(60), SNDH(60), SND(60),
3 SNDH(60), SND(60),
COMMON /DEBUG/ BEEC(12,60), BEEC(12,60), BEEC(12,60),
1 BEEC(12,60), BEEC(12,60), BEEC(12,60),
2 BEEC(12,60), BEEC(12,60), BEEC(12,60),
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X BEEC(12,60), BEEC(12,60), BEEC(12,60),
Y BEEC(12,60), BEEC(12,60), BEEC(12,60),
Z BEEC(12,60), BEEC(12,60), BEEC(12,60),
COMMON /SPEC/ MF, XMOL
DIMENSION XKT(60), DQ(60)

** BAND AVERAGE ABSORPTION CROSS SECTION (EQ. A2) **

SIGMA(ZH, ZA, ZB, ZG) = ((5.0E+03*TI*ZG*ZKZ)/BE) * (EXP(ZDL/TI)
1 *ZH*(ZA+ZB* (ZH**2)/3.0) +
2 *TI*(ZA+2.0*ZG*TI2) -TI*EXP((ZH-ZHVP)/TI)
3 *(ZA+ZB*(ZVHP-ZH)**2) -TI*EXP((ZH-ZHVP)/TI)
4 *2.0*ZB*TI*(ZHVP-ZH+TI))

SIGMA2(ZH, ZG, ZE, ZY) = 7.26E-16*TI*7ZG*EXP((-ZE-ZY)/T1)/ZH**3

GAMMA(ZX) = (1.0+ (1.5707963*ZX)**1.25)**(-0.4)

XLAMB(ZX) = (1.0+ZX*EXP(-ZX))/SQRT(1.0+6.283185*ZX)

** W(GROUP)/D CORRELATION (EQ. 88) **

PHI1(ZX) = (ATAN(1.570796*ZX)/1.570796)

** FLUX DIVERGENCE OVERLAPPING FUNCTION (EQ. 92) **

PHI2(ZX) = EXP(-ZX)

DO 400 I=1,NES
400 T(I) = T(I)*TD

ZHVP = 5.0

Y1 = 0.0

CONVER = 3.10375E+23*R*(I)*RDZ

SNDE(NES) = CONVER * C(7,NES)/SMW(7)

XNE = SNDE(NES)

FNE = (4.71E-6*XNE**2)/(T(NES)/11606)**1.0/7.0)

ZDL = AMIN(0, 20, FNE)

** DEBUG PRINT **

IF (IDG*NE.0) CALL BUGPR (1)
DELTA=W(1) * XL * 30.48006
CALL BUGPR (2)
6001 CONTINUE
DO 91 L=1, N
XKT(L)=T(L)/11606.
T1=XKT(L)
CALL SND(L)
C
C ** PARTITION FUNCTIONS FOR H, C, N, O **
C
94 IF(T(L)>15000.) GO TO 6
C
** LOW TEMPERATURE **
C
SUMH=2.0
SUMC =9.0 + 5.0 * EXP(-1.264/T1) + EXP(-2.684/T1) + 1
5.0 * EXP(-4.183/T1)
SUMN=4.0 + 10.0 * EXP(-2.384/T1) + 6.0 * EXP(-3.576/T1)
SUMO= 9.0 + 5.0 * EXP(-1.975/T1)
GO TO 7
C
C ** HIGH TEMPERATURE **
C
6 SUMH=2.0
SUMC=2.71818 + 6.40677 * T(L)/1.0E4 -0.45466 * (T(L)/1.0E4)**2
SUMN=5.938216 - 0.225593 * T(L)/1.0E3 + 0.015408 * (T(L)/1.0E3)**2
SUMO=11.79963 -0.317964 * T(L)/1.0E3 + 0.013765 * (T(L)/1.0E3)**2
CONTINUE
T12=T1**2
GH = 6.4994
DO 5 K=1, 12
GF=FVC(K)/T1
GHM=GH
GH=EXP(-GF) *GF * (GF**2 + 3.0 *GF +6.0 + 6.0/GF)
C
** PLANK MEAN ABSORPTION COEFFICIENT FOR BAND INTERVALS (EQ.A3) **  

\[ B(E)(K, L) = 5.04 \times 10^3 \times (T12**2) \times (GHM - GH) \]

\[ B(E) = B(E)(K, L) \]

** ABSORPTION CROSS SECTIONS **  

N

O

C

H

N2

O2

C2

H2

C0

C2H

C0

C3

\[ SGH = 0.0 \]
\[ SGN = 0.0 \]
\[ SGC = 0.0 \]
\[ SGO = 0.0 \]
\[ SGC0 = 0.0 \]
\[ SGC2 = 0.0 \]
\[ SGO2 = 0.0 \]
\[ SGN2 = 0.0 \]
\[ SGH2 = 0.0 \]
\[ SGC3 = 0.0 \]
\[ SGC2H = 0.0 \]

GO TO (581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594)

581 \[ SGH = \text{SIGMA}(2.41, 0.0, 0.1, 0) \times \exp(-13.56/T1) \]
\[ SGC = \text{SIGMA}(3.78, 0.3, 0.0488, 1.33) \times \exp(-11.26/T1) \]
\[ SGN = \text{SIGMA}(4.22, 0.24, 0.0426, 4.5) \times \exp(-14.54/T1) \]
\[ SGO = \text{SIGMA}(4.22, 0.24, 0.0426, 4.88) \times \exp(-13.61/T1) \]

GO TO 38

582 \[ ZZHV = 5.5 \]
\[ SGC2 = 8.0 \times 10^{-18} \times \exp(-0.5/T1) + 3.0 \times 10^{-18} \]
\[ SGC3 = 4.0 \times 10^{-18} \]

593 CALL ZHV(ZZHV, ZZN, ZZI, ZZC)
\[ SGC = \text{SIGMA2}(ZZHV, 1.03, 11.26, 3.78) \times ZZC + SGC \]
\[ SGN = \text{SIGMA2}(ZZHV, 4.50, 14.54, 4.22) \times ZZN \]
584 $Z_{HZV} = 7.5$
   $\text{SGC} = 5.0 \times 10^{-17} \times \exp\left(-4.18/T_1\right)/\text{SUMC}$
   $\text{SGCO} = 1.9 \times 10^{-17} \times \exp\left(-0.5/T_1\right)$
   $\text{SGC}_2 = 6.0 \times 10^{-19}$
   $\text{SGC}_3 = 3.0 \times 10^{-18}$
   $\exp\left(-0.7/11\right)$
   Go to 593

585 $Z_{HZV} = 8.5$
   $\text{SGC} = 5.0 \times 10^{-17} \times \exp\left(-4.18/T_1\right)/\text{SUMC}$
   $\text{SGCO} = 2.2 \times 10^{-17} \times \exp\left(-2.68/T_1\right)/\text{SUMC}$
   $\text{SGC}_2 = 2.2 \times 10^{-17}$
   $\text{SGC}_3 = 8.5 \times 10^{-19}$
   Go to 593

586 $Z_{HZV} = 9.5$
   $\text{SGC} = 5.0 \times 10^{-17} \times \exp\left(-4.18/T_1\right)/\text{SUMC}$
   $\text{SGCO} = 5.0 \times 10^{-17} \times \exp\left(-2.68/T_1\right)/\text{SUMC}$
   $\text{SGC}_2 = 1.0 \times 10^{-18}$
   $\text{SGC}_3 = 2.0 \times 10^{-17}$
   Go to 593

587 $Z_{HZV} = 10.5$
   $\text{SGN} = 3.2 \times 10^{-18} \times \exp\left(-0.2/T_1\right)/\text{SUMN}$
   $\text{SGO}_2 = 6.0 \times 10^{-19}$
   $Z_{HZV} = 10.5$
   Call ZHV($Z_{HZV}, Z_{ZO}, Z_{NZ}, Z_{ZI}, Z_{ZC}$)

588 $Z_{HZV} = 10.9$
   $\text{SGC} = (8.5 \times 10^{-17} \times \exp\left(-1.26/T_1\right) + 2.0 \times 10^{-17} \times \exp\left(-2.75/T_1\right)$
   $\times \exp\left(-4.18/T_1\right)/\text{SUMC}$
   Go to 594

589 $Z_{HZV} = 11.6$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38

590 $Z_{HZV} = 12.8$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38

591 $Z_{HZV} = 14.2$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38

592 $Z_{HZV} = 15.6$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38

593 $Z_{HZV} = 17.0$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38

594 $Z_{HZV} = 18.8$
   $\text{SGO} = \Sigma_{i=1}^{\infty} a_i \exp\left(-b_i/T_1\right)$
   Go to 38
SGN=(5.16E-17 * EXP(-3.50/T1))/SUMN
GO TO 596

589 ZZHV=11.6
CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)
SGN2=1.0F-18
SGN=(5.16E-17 * EXP(-3.50))/SUMN

598 SGC=(9.9E-17 + 8.5E-17 * EXP(-1.26/T1) + 2.2E-17 * EXP(-2.75/T1)) / SUMC

IF (K<LT11) GO TO 594
GO TO 38

590 ZZHV=12.7
CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)
SGN2=2.0F-18
SGH2=2.7E-17

599 SGN=(6.4E-17 * EXP(-2.30/T1) + 5.1E-17 * EXP(-3.50/T1))/SUMN
GO TO 598

591 SGH=1.18F-17/SUMH
SGO=3.6E-17/SUMO
SGN2=1.0E-17
SGH2=2.7E-17
GO TO 599

592 SGN=3.6E-17/SUMN
SGN2=1.0E-18
GO TO 599

CONTINUE

38 FMUC(K,L)= SNDH(L)*SGH + SNDC(L)*SGC + SNDN(L)*SGN + SNDO(L)*SGO
        + XMOL * (SNDC2(L)*SGN2 + SNDO2(L)*SGO2 +
        SNDC2(L)*SGC2 + SNDC2H(L)*SGC2H )

IF (L<GT1) GO TO 8
TAUC(K,L)=0.
GO TO 5

8 TAUC(K,L)=TAUC(K,L-1)+(YD(L)-YD(L-1))*FMUC(K,L-1)+FMUC(K,L)) * DELTA
5 CONTINUE
  IF (LINES .EQ. 0) GO TO 91
  C** FRACTIONAL POPULATION STATES FOR H, N, O, C **
  C
  CALL ZP (T1, SUMN, SUMO, SUMH, SUMC)
  C** CALCULATION OF PARAMETERS FOR 9 LINE GROUPES **
  C
  WN -- NUMBER OF LINES
  C
  FG -- EFFECTIVE F-NUMBER
  C
  GP -- EFFECTIVE HALF-WIDTH
  C
  GROUP 1
  C
  FG(1.2) = (1.02 * ZPC(5) + .795 * ZPC(6) + 0.114 * ZPC(7)) / WN(1.2)
  GP(1.2) = (8.16E-11 * SQRT(ZPC(5)) + 1.25E-10 * SQRT(ZPC(6))
  + 2.55E-10 * SQRT(ZPC(7))**2) / (FG(1.2) * WN(1.2)**2)
  FG(1.3) = (1.040 * ZPN(4) + 1.29 * ZFN(5) + 0.00 * ZPN(6)) / WN(1.3)
  GP(1.3) = (6.65E-11 * SQRT(ZPN(4)) + 1.71E-10 * SQRT(ZPN(5))
  + 9.00E-10 * SQRT(ZPN(6))**2) / (FG(1.3) * WN(1.3)**2)
  FG(1.4) = (1.00 * ZPO(4) + .978 * ZPO(5)) / WN(1.4)
  GP(1.4) = (3.90E-11 * SQRT(ZPO(4)) + 9.68E-11 * SQRT(ZPO(5))**2) / (FG(1.4) * WN(1.4)**2)
  FMUL(1,L) = FMUC(1,L)
  C
  GROUP 2
  C
  FG(2.1) = 0.805 * ZPH(2) / WN(2.1)
  GP(2.1) = 2.37E-10 * 2.37E-10 * ZPH(2) / (FG(2.1) * WN(2.1)**2)
  FG(2.2) = (0.00E-2 * ZPC(5) + 6.71E-2 * ZPC(6)) / WN(2.2)
  GP(2.2) = (0.00E-12 * SQRT(ZPC(5)) + 7.15E-11 * SQRT(ZPC(6))**2)
  + 2.85E-2 * ZPN(5)) / WN(2.3)
  GP(2.3) = (1.11E-10 * SQRT(ZPN(4)) + 6.07E-11 * SQRT(ZPN(5))**2)
  + 8.25E-2 * ZPO(5)) / WN(2.4)
  GP(2.4) = (2.61E-11 * SQRT(ZPO(4)) + 7.19E-11 * SQRT(ZPO(5))**2)
1  /(FG(2,4) * WN(2,4)**2)  
FMUL(2,L)=FMUC(1,L)

C GROUP 3
FG(3,2)=(7.29E-2 * ZPC(2) + 6.76E-2 * ZPC(3))/WN(3,2)
GP(3,2)=(9.08E-12 * SQRT(ZPC(2)) + 8.75E-12 * SQRT(ZPC(3)))**2
1  /(FG(3,2) * WN(3,2)**2)  
FMUL(3,L)=FMUC(2,L)

C GROUP 4
FG(4,2)=(1.05 * ZPC(1) + 1.10E-2 * ZPC(2) + 0.150 * ZPC(3))/WN(4,2)
GP(4,2)=(9.57E-12 * SQRT(ZPC(1)) + 4.86E-12 * SQRT(ZPC(2)))**2/(FG(4,2) * WN(4,2)**2)  
FG(4,2)=(7.40E-2 * ZPN(2) + 6.34E-2 * ZPN(3))/WN(4,3)
GP(4,3)=(8.22E-12 * SQRT(ZPN(2)) + 7.60E-12 * SQRT(ZPN(3)))**2  
1  /(FG(4,3) * WN(4,3)**2)  
FMUL(4,L)=FMUC(4,L)

C GROUP 5
FG(5,2)=(0.329 * ZPC(1) + 0.118 * ZPC(2) + 0.226 * ZPC(4))/WN(5,2)
GP(5,2)=(3.05E-11 * SQRT(ZPC(1)) + 5.77E-10 * SQRT(ZPC(2)))**2/(FG(5,2) * WN(5,2)**2)  
FG(5,3)=0.108 * ZPN(3)/WN(5,3)
GP(5,3)=3.09E-11 * 3.09E-11 * ZPN(3)/(FG(5,3) * WN(5,3)**2)
FG(5,4)=4.71E-2 * ZPN(1)/WN(5,4)
FG(5,4)=5.08E-12 * 5.08E-12 * ZPN(1)/(FG(5,4) * WN(5,4)**2)  
FMUL(5,L)=FMUC(4,L)

C GROUP 6
FG(6,1)=0.416 * ZPH(1)/WN(6,1)
GP(6,1)=3.02E-11 * 3.02E-11 * ZPH(1)/(FG(6,1) * WN(6,1)**2)
FG(6,2)=8.65E-7 * ZPC(1)/WN(6,2)
GP(6,2)=2.35E-10 * 2.35E-10 * ZPC(1)/(FG(6,2) * WN(6,2)**2)  
FG(6,3)=(0.164 * ZPN(1) + 0.29C * ZPN(2) + 8.52E-2 * ZPN(3))/WN(6,3)
1  /(WN(6,3))  
GP(6,3)=(1.07E-11 * SQRT(ZPN(1)) + 4.28E-11 * SQRT(ZPN(2)))**2/(FG(6,3) * WN(6,3)**2)  
1  + 2.09E-10 * SQRT(ZPN(3))**2/(FG(6,3) * WN(6,3)**2)  
FMUL(6,L)=FMUC(6,L)
\[
FG(6.4) = (0.120 \cdot ZPO(2) + 0.151 \cdot ZPO(3)) / WN(6.4) \\
GP(6.4) = (8.85E-12 \cdot \text{SQRT}(ZPO(2)) + 9.93E-12 \cdot \text{SQRT}(ZPO(3))) / WN(6.4) \\
\]

\[
1 / (FG(6.4) \cdot WN(6.4) ^ 2) \\
FMUL(6.4) = FMUC(7.4) \\
\]

\[C_{\text{GROUP 7}}\]

\[
FG(7.2) = (4.51E-2 \cdot ZPC(1) + 9.66E-2 \cdot ZPC(2)) / WN(7.2) \\
GP(7.2) = (6.07E-10 \cdot \text{SQRT}(ZPC(1)) + 2.34E-10 \cdot \text{SQRT}(ZPC(2))) / WN(7.2) \\
\]

\[1 / (FG(7.2) \cdot WN(7.2) ^ 2) \\
FG(7.3) = (0.454 \cdot ZPN(1) + 0.178 \cdot ZPN(3)) / WN(7.3) \\
GP(7.3) = (2.71E-12 \cdot \text{SQRT}(ZPN(1)) + 8.37E-12 \cdot \text{SQRT}(ZPN(2))) / WN(7.3) \\
\]

\[1 / (FG(7.3) \cdot WN(7.3) ^ 2) \\
FG(7.4) = (0.23E-2 \cdot ZPO(2) / WN(7.4) \\
GP(7.4) = (2.52E-11 \cdot ZPO(2) / WN(7.4) \\
\]

\[FMUL(7.4) = FMUC(8.4) \\
\]

\[C_{\text{GROUP 8}}\]

\[
FG(8.1) = (0.108 \cdot ZPH(1)) / WN(8.1) \\
GP(8.1) = (1.32E-10 \cdot ZPH(1)) / WN(8.1) \\
\]

\[1 / (FG(8.1) \cdot WN(8.1) ^ 2) \\
FG(8.2) = (0.379 \cdot ZPC(1) + 1.05 \cdot ZPC(3)) / WN(8.2) \\
GP(8.2) = (1.95E-11 \cdot \text{SQRT}(ZPC(1)) + 1.27E-10 \cdot \text{SQRT}(ZPC(3))) / WN(8.2) \\
\]

\[1 / (FG(8.2) \cdot WN(8.2) ^ 2) \\
FG(8.3) = (0.165 \cdot ZPN(1) + 0.142 \cdot ZPN(2) + 3.75E-2 \cdot ZPN(3)) / WN(8.3) \\
\]

\[1 / (FG(8.3) \cdot WN(8.3) ^ 2) \\
GP(8.3) = (2.98E-11 \cdot \text{SQRT}(ZPN(1)) + 7.08E-11 \cdot \text{SQRT}(ZPN(2))) / WN(8.3) \\
\]

\[1 / (FG(8.3) \cdot WN(8.3) ^ 2) \\
FG(8.4) = (0.146 \cdot ZPO(1) + 8.61E-2 \cdot ZPO(2)) / WN(8.4) \\
GP(8.4) = (1.97E-10 \cdot \text{SQRT}(ZPO(1)) + 1.89E-11 \cdot \text{SQRT}(ZPO(2))) / WN(8.4) \\
\]

\[1 / (FG(8.4) \cdot WN(8.4) ^ 2) \\
FMUL(8.4) = FMUC(9.4) \\
\]

\[C_{\text{GROUP 9}}\]

\[
FG(9.2) = (2.95 \cdot ZPC(2)) / WN(9.2) \\
GP(9.2) = (5.85E-12 \cdot ZPC(2)) / WN(9.2) \\
\]

\[FG(9.3) = (0.224 \cdot ZPN(1) + 2.92E-2 \cdot ZPN(2)) / WN(9.3) \\
\]

\[FMUL(9.3) = FMUC(10.3) \\
\]
GP(9,3) = (3.41E-10 * SQRT(ZPN(1)) + 1.48E-10 * SQRT(ZPN(2)))**2

FG(9,4) = (5.24E-2 * ZPO(1) + 7.22E-2 * ZPO(2))

GP(9,4) = (5.76E-12 * SQRT(ZPO(1)) + 7.20E-11 * SQRT(ZPO(2)))**2

TRAN3160

1

TRAN3170

FG(9,4) = (5.24E-2 * ZPO(3))/WN(9,4)

TRAN3180

GP(9,4) = (5.76E-12 * SQRT(ZPO(1)) + 7.20E-11 * SQRT(ZPO(2)))**2

TRAN3190

FMUL(9,L) = FMULC(11,L)

TRAN3200

C

TRAN3210

C ** PLANCK FUNCTION **

C

DO 9 J=1,NHVL

BEEL(J,L) = 5.04E3 * HVJ(J)**3 / (EXP(HVJ(J)/T1) - 1.0)

TRAN3220

C

TRAN3230

C ** INDUCED EMISSICN FACTOR (EQ 81) **

C

SSM(J,1,L) = 1.10E-16 * SNDH(L) * (1.0 - EXP(-HVJ(J)/T1)) * FG(J,1)

TRAN3240

SSM(J,2,L) = 1.10E-16 * SNDC(L) * (1.0 - EXP(-HVJ(J)/T1)) * FG(J,2)

TRAN3250

SSM(J,3,L) = 1.10E-16 * SNDN(L) * (1.0 - EXP(-HVJ(J)/T1)) * FG(J,3)

TRAN3260

SSM(J,4,L) = 1.10E-16 * SNDO(L) * (1.0 - EXP(-HVJ(J)/T1)) * FG(J,4)

TRAN3270

DO 10 M=1,4

GGM(J,M,L) = GP(J,M) * SNDE(L) * (T(L)/1.0E4)**0.25

TRAN3280

1 + 1.0E-6

IF(L*GT.1) GO TO 11

ETAM(J,M,L-1) = 0

SBM(J,M,L) = 0

GO TO 10

11 ETAM(J,M,L,L) = ETAM(J,M,L-1) + (YD(L) - YD(L-1))

1 * (SSM(J,M,L-1) * GGM(J,M,L-1) + SSM(J,M,L) * GGM(J,M,L))

TRAN3290

* DELTA/3.14159265

TRAN3300

SBM(J,M,L) = SBM(J,M,L-1) + (YD(L) - YD(L-1))

TRAN3310

1 * (SSM(J,M,L-1) + SSM(J,M,L)) * DELTA

TRAN3320

10 CONTINUE

IF (L*GT.1) GO TO 12

TAUL(J,1) = 0

GO TO 9

TRAN3330

TRAN3340

TRAN3350

TRAN3360

TRAN3370

TRAN3380

TRAN3390

TRAN3400

TRAN3410

TRAN3420

TRAN3430

TRAN3440

TRAN3450

TRAN3460

TRAN3470

TRAN3480

TRAN3490

TRAN3500
12 TAUL(J,L) = TAUL(J,L-1) + (YD(L)-YD(L-1))
   * (FMUL(J,L-1)+FMUL(J,L)) * DELTA
     CONTINUE
   IF (IDGoNEo99) GO TO 91
   CALL BUGPR (7)

9 CONTINUE
   IEZ=IEZ+1
   ETZ(IEZ)=1.0

** CONTINUUM - CONTINUUM FLUX DIVERGENCE CALCULATION **

C

DO 3CO K=1,IEZ
   DO 31 LK=INES
      I=LK
      NUT(K)=I
      IF (ABS(ETZ(K)-ETA(LK)) - 1.0E-5) 300,300,31
   31 CONTINUE

300 CONTINUE
   DO 1612 J=1,9
      OCLP(J)=0.0
      QLCP(J)=0.0
      QLLP(J)=0.0
   1612 FP(J,L)=0.0
   DO 1613 L=1,INES
      FM(J,L)=0.0
   1613 FL(L)=0.0
   DO 49 IYY=1,IEZ
      IY=NUT(IYY)
   49 CONTINUE
   DO 20 K=1,12
      FMC(K,IY)=0.0
      FPC(K,IY)=0.0
IF (IY.EQ.1) GO TO 44
DO 40 L=1,IY
C ** MINUS EMISSIVITY FUNCTION (EQ 47) *
C EM(K*L)=1.0 - EXP(TAUC(K,L)-TAUC(K,IY))
IF (L.EQ.1) GO TO 40
C ** MINUS CONTINUUM FLUX (EQ 46) **
C FMC(K,IY)=FMC(K,IY) - (EM(K,L)-EM(K,L-1))
   * (BEEC(K*L-1)+BEEC(K,L))/2.
40 CONTINUE
44 IF (IY.EQ.NES ) GO TO 41
DO 42 L=1,Y,NES
C ** POSITIVE EMISSIVITY FUNCTION (EQ 47) **
C EP(K*L)=1.0 - EXP(TAUC(K,IY)-TAUC(K,L))
IF (L.EQ.IY) GO TO 42
C ** POSITIVE EMISSIVITY CONTINUUM FLUX (EQ 46) **
C FPC(K,IY)=FPC(K,IY) + (EP(K,L)-EP(K,L-1))
   * (BEEC(K*L-1)+BEEC(K,L))/2.
42 CONTINUE
C ** POSITIVE EMISSIVITY CONTINUUM FLUX DIVERGENCE (EQ 51) **
C 41 QCCP(K)=6.2831853 * FMUC(K,IY) *
   * (FMC(K,IY) + FPC(K,IY) - 2.0* BEEC(K,IY))
   * FMUC(K,IY) = FMUC(K,IY) * 2.14159265
   * FPC(K,IY) = FPC(K,IY) * 2.14159265
20 CONTINUE
C ** DEBUG PRINT **
C
IF (IDG.NE.99) GO TO 21
CALL BUGPR (3)
21 QCC(IYY)=0.
DO 24 K=1,12
C
C ** LINE AND CROSS TERM FLUX DIVERGENCE CALCULATION **
C
24 QCC(IYY)=QCC(IYY) + QCCP(K)
IF (LINES.EQ.0) GO TO 1E14
C
C ** INTEGRATION FROM 1 TO IY **
C
IF (IY.EQ.1) GO TO 68
DO 65 J=1,9
DO 66 L=1,IY
WIM=0.
SUM1=0.
SUM2=0.
DO 67 M=1,4
DIF=ETAM(J,M,IY) - ETAM(J,M,L)
DIFSBM = SBM(J,M,IY)-SBM(J,M,L)
IF (ABS(DIFSBM).LT.1.E-10) DIFSBM = 1.E-10
BETAM=DIF / ( DIFSBM ) * 3.14159265
IF (L.EQ.I) BETAM=GGM(J,M,L)
IF (ABS(DIF).GT.1.E-10) GO TO 9001
TM = 1.E-10
GO TO 9002
9001 CONTINUE
TM=DIF /2.0/BETAM**2
9002 RRMM=DIF/2.0/GGM(J,M,IY)**2
WWMM=6.2831853 * WN(J,M) * BETAM * GAMMA(TM) * TM
SUM1=SUM1 + GAMMA(TM) * WN(J,M) * SSM(J,M,IY)
SUM2=SUM2 + XLAMB(RFM) * WN(J,M) * SSM(J,M,IY)
** OVERLAPPING LINE CALCULATIONS **

** GROUP EQUIVALENT WIDTHS (EQ.88) **

\[ \text{WMM}(J,L) = DJ(J) \times \text{PHII}(\text{ALPHAM}) \times \exp(\text{Taul}(J,L) - \text{Taul}(J,IY)) \]

** GROUP GAMMA -- LINE TRANSPORT FUNCTION (EQ.92) **

\[ \text{GMM}(J,L) = \text{PHI2}(\text{ALPHAM}) \times \text{SUM1} \]

** MINUS EMISSIVITY FUNCTION FOR LINES (EQ.47) **

\[ \text{EFM}(J,L) = 1.0 - \exp(\text{Taul}(J,L) - \text{Taul}(J,IY)) \]

CONTINUE

IF (IDG.EQ.99) CALL BUGPR(1)
IF (IDG.EQ.99) CALL BUGPR(4)

IF (IY.EQ.NES) GO TO 72

** INTEGRATION FROM IY TO NES **

\[ \text{DIF} = \text{ETAM}(J,M,L) - \text{ETAM}(J,M,IY) \]
\[ \text{DIFSBM} = \text{SBM}(J,M,L) - \text{SBM}(J,M,IY) \]
\[ \text{IF}(\text{ABS}(\text{DIFSBM}) \cdot \text{LT} \cdot 10^{-10}) \quad \text{DIFSBM} = 10^{-10} \]
\[ \text{BETAP} = \text{DIF} / (\text{DIFSBM}) \times 3.14159265 \]
IF (L.EQ.IY) BETAP=GGM(J,M,L)

IF (ABS(DIF).GT.1.E-10) GO TO 9003

TP = 1.E-10

GO TO 9004

9003 CONTINUE

TP=DIFF/2.O/BETAP**2

9004 RRP=DIFF/2.O/GGM(J,M,IY)**2

WIP=2831853 * WN(J,M) * BETAP * GAMMA(TP) * TP

SUM1=SUM1 + GAMMA(TP) * WN(J,M) * SSM(J,M,IY)

SUM2=SUM2 + XLAMB(RFP) * WN(J,M) * SSM(J,M,IY)

71 WIP=WIP+WIP

ALPHAP=WIP/DJ(J)

WPP(J,L)=DJ(J) * PHI1(ALPHAP) * EXP(TAUL(J,IY)-TAUL(J,L))

GPP(J,L)=PHI2(ALPHAP) * SUM1

C ** POSITIVE EMISSIVITY FUNCTION FOR LINES (EQ*47) **

EEP(J,L)=1.0 - EXP(TAUL(J,IY)-TAUL(J,L))

70 XLPP(J,L)=PHI2(ALPHAP) * SUM2

69 CONTINUE

C ** DEBUG PRINT **

IF (IDG.EQ.99) CALL BUGPR (5)

C 72 DO 80 J=1,9

ASM1=0.

ASM2=0.

FM(J,IY)=0.

IF (IY.EQ.1) GO TO 81

DO 82 L=2,IY

FM(J,IY)=FM(J,IY) - (WMM(J,L)-WMM(J,L-1))

1 *(BEEL(J,L-1)+BEEL(J,L)) * 1.5707963

IF (L.EQ.IY) GO TO 82

ASM1=ASM1 - (EEP(J,L)-EEP(J,L-1))

1 *(BEEL(J,L-1) * XLMM(J,L-1) + BEEL(J,L) * XLMM(J,L))/2.

82 CONTINUE

80 CONTINUE

C
ASM2=ASM2 - (XLM(J,L)-XLM(J,L-1))
1 * (BEEL(J,L-1) * EXP(TAUL(J,L-1)-TAUL(J,IY)) + BEEL(J,L))
2 * EXP(TAUL(J,L)-TAUL(J,IY)) / 2.0

82 CONTINUE

81 ASP1=0.
ASP2=0.
IYP=IY+1
IF (IY.EQ.NES) GO TO 83
DO 84 L=IYP,NES
FP(J,IY)=FP(J,IY) + (WPP(J,L)-WPP(J,L-1))
1 * (BEEL(J,L-1)+BEEL(J,L)) * 1.5707963
IF (L.EQ.IYP) GO TC 84
ASP1=ASP1 + (EEP(J,L)-EEP(J,L-1))
ASP2=ASP2 + (XLPP(J,L-1)-XLPP(J,L-1))
1 * (BEEL(J,L-1) * EXP(TAUL(J,IY)-TAUL(J,L-1)) + BEEL(J,L))
2 * EXP(TAUL(J,IY)-TAUL(J,L)) / 2.0

84 CONTINUE

83 QLCP(J)=2.0 * FMUL(J,IY) * (FM(J,IY)+FP(J,IY))
SUMS=1.0
SUMT=0.0
DO 86 M=1,4
SUMT=SUMT + SSM(J,M,IY) * WN(J,M)
ATMI=0.
IF (IY.NE.1) ATMI=(BEEL(J,IY-1)+BEEL(J,IY)) / 2.0 * EEM(J,IY-1)
1 * XLM(J,IY-1)
ATPI=0.
IF (IY.NE.NES) ATPI=(BEEL(J,IY+1)+BEEL(J,IY)) / 2.0 * EEP(J,IY+1)
1 * XLPP(J,IY+1)
QLCP(J)=6.2831853 * SUMS * (ASM1+ASP1+ATM1+ATP1)
IF (IY.EQ.1) ATRM2=-BEEL(J,IY) * SUMT
IF (IY.NE.1) ATRM2=(BEEL(J,IY-1)-BEEL(J,IY)) * GMM(J,IY-1)
1 - BEEL(J,IY-1) * XLM(J,IY-1)
IF (IY.EQ.NES) ATP2=-BEEL(J,IY) * SUMT
IF (IY.NE.NES) ATP2=(BEEL(J,IY+1)-BEEL(J,IY)) * GPP(J,IY+1)
1 - BEEJ(J, IY+1) * XLPP(J, IY+1)

QLLP(J) = 6.2831 * SUMS*(-ASM2-ASP2+ATM2+ATP2)

80 CONTINUE

QCL(IYY) = 0
QLC(IYY) = 0
QLL(IYY) = 0

DO 85 J=1,9

QCL(IYY) = QCL(IYY) + QCLP(J)
QLC(IYY) = QLC(IYY) + QLCP(J)
QLL(IYY) = QLL(IYY) + QLLP(J)

1614 CONTINUE

DQN(IYY) = -(QCC(IYY) + QCL(IYY) + QLC(IYY) + QLL(IYY))

C
C ** DEBUG PRINT **
C

IF (IDG.EQ.0) GO TO 49
CALL BUGPR(6)

49 CONTINUE

IEZ = IEZ - 1
D0(1) = DQN(1)
L = 2

DO 1 N=2, NES
DO 2 I=2, IEZ

NP = I
IF (ETZ(I) .GT. ETA(N)) GO TO 3

2 CONTINUE

3 NN = NP - 1

AA = 0
ZB = (DQN(NN) - DQN(NP)) / (ETZ(NN) - ETZ(NP))
CC = DQN(NN) - ZB * ETZ(NN)
DQ(N) = AA * ETA(N) ** 2 + ZB * ETA(N) + CC
GO TO 1

4 DQ(N) = DQN(NN)
1 CONTINUE
** Non-Dimensionalize E(I) **
DO 250 I=1,NES
   T(I) = T(I)/TD
250   E(I) = ((DQ(I)*XL)/(RINF*UINF**3))*20866.0 *RZB
RETURN
END
SUBROUTINE TRANS2
COMMON /SFLUX/ QRI(3)
COMMON /YL/ETA(60), YOND(60)
COMMON /FRSTRM/ UINF, RINF, UINF2, R, RE, LXI, ITN, IEM, NES
COMMON /TRN/ NUT(60), FMC(12,60), FPC(12,60),
1 FM(9,60), FP(9,60), LINES
COMMON /FINV/ NHVL, NIHVC, FHVC(12), DJ(9), HVJ(9), ZKZ
COMMON /TEST/ ETA(60), IEZ
COMMON /NUMDEN/ SND02(60), SNDN2(60), SNDQ(60), SNDN(60),
1 SNDH(60), SNDC2(60), SNDH2(60), SNDCO(60),
2 SNDC3(60), SNDC2H(60)
COMMON /SPEC/ MF, XMOL
DIMENSION ETOUT(3)
NETA=NES
ETOUT(1)=0.0
ETOUT(2)=0.5
ETOUT(3)=1.0
NOUT=3

C
C OUTPUT FLUX
C
WRITE (6,600)
WRITE (6,603) (ETA(I), SND2(I), SND02(I), SNDQ(I), SNDN(I),
1 SNDE(I), SNDH(I),
2 SNDC(I), SNDC2(I), SNDH2(I), SNDCO(I), SNDC3(I),
3 SNDC2H(I), I=1, NETA)

C ** CONTINUUM CONTRIBUTION TO THE SPECTRAL FLUX **
C
WRITE (6,4133)
DO 8040 K=1, NOUT
DO 8041 LK=1, NES
NUT(K)=LK
IF (ABS(ETOUT(K)-ETA(LK)) - 1.0E-05) 8040, 8040, 8041
8041 CONTINUE
8040 CONTINUE
   LI=NUT(1)
   L2=NUT(2)
   L3=NUT(3)
   WRITE (6,8037) (ETGUT(IL),IL=1,3)
   FM1=0.0
   FP1=0.0
   FM2=0.0
   FP2=0.0
   FM3=0.0
   FP3=0.0
   DO 4104 KL=1,NIHVC
   WRITE (6,8042) KL, FHVC(KL), FMC(KL,L1), FPC(KL,L1),
   FMC(KL,L2), FPC(KL,L2), FMC(KL,L3), FPC(KL,L3)
   FM1=FM1 + FMC(KL,L1)
   FP1=FP1 + FPC(KL,L1)
   FM2=FM2 + FMC(KL,L2)
   FP2=FP2 + FPC(KL,L2)
   FM3=FM3 + FMC(KL,L3)
   FP3=FP3 + FPC(KL,L3)
   4104 CONTINUE
   WRITE (6,8045) FM1, FP1, FM2, FP2, FM3, FP3
   QRI(1)=FM1+FP1
   QRI(2)=FM2+FP2
   QRI(3)=FM3+FP3
   C** LINE CONTRIBUTION TO THE SPECTRAL FLUX **
   C
   IF (LINES.EQ.0) RETURN
   WRITE (6,8035)
   WRITE (6,8037) (ETGUT(IL),IL=1,3)
   FM1=0.0
   FP1=0.0
   FM2=0.0
   FP2=0.0
   TRAN 360
   TRAN 370
   TRAN 380
   TRAN 390
   TRAN 400
   TRAN 410
   TRAN 420
   TRAN 430
   TRAN 440
   TRAN 450
   TRAN 460
   TRAN 470
   TRAN 480
   TRAN 490
   TRAN 500
   TRAN 510
   TRAN 520
   TRAN 530
   TRAN 540
   TRAN 550
   TRAN 560
   TRAN 570
   TRAN 580
   TRAN 590
   TRAN 600
   TRAN 610
   TRAN 620
   TRAN 630
   TRAN 640
   TRAN 650
   TRAN 660
   TRAN 670
   TRAN 680
   TRAN 690
   TRAN 700
FM3=0.0
FP3=0.0

** TOTAL FLUX CALCULATION **

DO 8043 KL=1,NHLV
WRITE (6,8042) KL, HVJ(KL), FM(KL,L1), FP(KL,L1).
1 FM(KL,L2), FP(KL,L2), FM(KL,L3), FP(KL,L3)
FM1=FM1 + FM(KL,L1)
FP1=FP1 + FP(KL,L1)
FM2=FM2 + FM(KL,L2)
FP2=FP2 + FP(KL,L2)
FM3=FM3 + FM(KL,L3)
FP3=FP3 + FP(KL,L3)
CONTINUE
8043 WRITE (6,8043) FM1, FP1, FM2, FP2, FM3, FP3
QRI(1)=QRI(1) + FM1 + FP1
QRI(2)=QRI(2) + FM2 + FP2
QRI(3)=QRI(3) + FM3 + FP3
600 FORMAT (1H1, 3H NUMBER DENSITIES (PARTICLES/CN3) /// 5X, 3HETA, 8X)
1 2H2N2, 8X, 2H2O2, 8X*1HN, 8X*1HC, 8X, 2HE/, 8X,
2 1HM, 8X, 1HC, 8X*2HC2, 8X*2HM2, 8X*2HC0, 8X*2HC3, 8X, 3HC2H////)
603 FORMAT (1P13E10.2)
4103 FORMAT (44H CONTINUUM CONTRIBUTION TO THE SPECTRAL FLUX)
8035 FORMAT (39H LINE CONTRIBUTION TO THE SPECTRAL FLUX)
8037 FORMAT (72X, 5HETA =F7.3, 13X, 5HETA =F7.3, 13X, 5HETA =F7.3, 13X, 1H1)
1 3X, 3HMNU, 8X, 6HMINUS, 7X, 5HPLUS, 8X, 6HMINUS, 7X, 5HPLUS, 8X,
2 6HMINUS, 7X, 5HPLUS//)
8042 FORMAT (I4, F8.3, 1PEE13.3)
8045 FORMAT (12H TOTAL FLUX , 1P8E13.3)
RETURN
END
SUBROUTINE SND(I)
COMMOM/PROP1/PI(60),RHO(60), T(60),AMW(60),C (20,60),EC(5,60)
COMMOM/RFLUX/ E(60),IRAD,ITYPE
COMMOM/NON/RDZ*MUDZ,RMDZ,AKNF,HNF,CFNF
COMMOM/WT/SMW(20),AWT(5)
COMMOM/NUMDEN/ SND02(60), SNDN2(60), SND(60), SNDN(60),
1 SNDHE(60), SND(60),
2 SNDH(60), SND2C(60), SNDHE2(60), SND(60),
3 SNDC3(60), SND(60)

1 *
2 *
3 *

C ** CALCULATE SPECIE NUMBER DENSITIES BASED ON MOLE FRACITIONS **
C
C CONVER = 3.10375E+23 *RHO(I) *RDZ
C
SNDO2(I) = CONVER * C( 1,I)/SMW( 1)
SND2(I) = CONVER * C( 2,I)/SMW( 2)
SNDD(I) = CONVER * C( 3,I)/SMW( 3)
SNDN(I) = CONVER * C( 4,I)/SMW( 4)
SNDN2(I) = CONVER * C( 7,I)/SMW( 7)
SNDH(I) = CONVER * C( 8,I)/SMW( 8)
SNDH2(I) = CONVER * C(10,I)/SMW(10)
SNDCO(I) = CONVER * C(11,I)/SMW(11)
SND2C(I) = CONVER * C(12,I)/SMW(12)
SND2H(I) = CONVER * C(19,I)/SMW(19)
SND2H2(I) = CONVER * C(14,I)/SMW(14)

RETURN
END
SUBROUTINE ZP(T1, SUMN, SUMO, SUMH, SUMC)

** FRACTIONAL POPULATION STATES FOR N, O, H, C **

COMMON /ZPI/ ZPO(6), ZPN(6), ZPH(2), ZPC(7)

ZPH(1) = 2.0 / SUMH
ZPH(2) = 8.0 * EXP(-1.02/T1) / SUMH
ZPC(1) = 9.0 / SUMC
ZPC(2) = 5.0 * EXP(-1.264/T1) / SUMC
ZPC(3) = EXP(-2.684/T1) / SUMC
ZPC(4) = 5.0 * EXP(-4.183/T1) / SUMC
ZPC(5) = 12.0 * EXP(-7.532/T1) / SUMC
ZPC(6) = 36.0 * EXP(-8.722/T1) / SUMC
ZPC(7) = 60.0 * EXP(-9.724/T1) / SUMC
ZPN(1) = 4.0 / SUMN
ZPN(2) = 10.0 * EXP(-2.384/T1) / SUMN
ZPN(3) = 6.0 * EXP(-3.576/T1) / SUMN
ZPN(4) = 18.0 * EXP(-10.452/T1) / SUMN
ZPN(5) = 54.0 * EXP(-11.877/T1) / SUMN
ZPN(6) = 90.0 * EXP(-13.002/T1) / SUMN
ZPO(1) = 9.0 / SUMO
ZPO(2) = 5.0 * EXP(-1.967/T1) / SUMO
ZPO(3) = EXP(-4.188/T1) / SUMO
ZPO(4) = 8.0 * EXP(-9.283/T1) / SUMO
ZPO(5) = 24.0 * EXP(-10.830/T1) / SUMO
ZPO(6) = 40.0 * EXP(-12.077/T1) / SUMO

RETURN

END
SUBROUTINE BUGPR (IDGSW)

COMMON /FRSTRM/ U INF, RINF, UINF2, R, RE, LXI, ITM, IEM, NES

COMMON /YL/ETA(60), YD(60)

COMMON /TRN/ NUT(60), FMC(12,60), FPC(12,60),

1 FM(9,60), FP(9,60), LINES

COMMON /DEBUG/ QLC(60), QCL(60), QLL(60), QDN(60), QCC(60),

1 BEEC(12,60), FMUC(12,60), EM(12,60),

2 EP(12,60), TAUC(12,60), BEEL(9,60),

3 QCCP(12), WMM(9,60), GMM(9,60),

4 EEM(9,60), XLMM(9,60), OLCP(9),

5 QCL(9), QLPP(9), DELTA, IY, IYY,

6 WPP(9,60), GPP(9,60), EEP(9,60),

7 XLPP(9,60), FG(9,4), GP(9,4),

8 WNN(9,4), FMUL(9,60), SSM(9,4,60),

9 GGM(9,4,60), ETAM(9,4,60), SBM(9,4,60),

A TAUL(9,60),

GO TO (10,20,30,40,50,60,70), IDGSW

10 WRITE (6,194)

194 FORMAT (IH1)

RETURN

WRITE (6,7182) DELTA

7182 FORMAT (7H0DELTA=1PE14.7,3H CM)

RETURN

30 WRITE (6,196) IY, YD(IY)

190 FORMAT (4H11Y=13,2X,3HYD=1PE12.5,/2X,1HK,2X,1HL,7X,3HETA,13X,2HYD)

1 13X,2HMU,11X,3HTAU,14X,1HE,11X,3HBEE/>

DO 22 K=1,12

22 IF (IY.EQ.1) GO TO 23

WRITE (6,191) (K, EM(K,L), ETA(L), YD(L), FMUC(K,L), TAUC(K,L),

1 EM(K,L), BEEC(K,L), L=1,IY)

191 FORMAT (2I3,1PE15.5)

WRITE (6,192)

192 FORMAT (/)

23 IF (IY.EQ.NES) GO TO 22

WRITE (6,191) (K, ETA(L), YD(L), FMUC(K,L),

1 200,210,220,230,240,250,260,270,280,290,300,310,320,330,340,350
1  TAUC(K,L), EP(K,L), BEEC(K,L), L=IY, NES) BUGP 360
22 WRITE (6,193) FMC(K,IY), FPC(K,IY), QCCP(K)
193 FORMAT (5H0F=IPE12.5, 2X, 4HFIP=E12.5, 2X, 5HCCP=E12.5) BUGP 370
  RETURN

19  WRITE (6,195) IY, YD(IY), ((J, L, YD(L), BUGP 400
1  WMM(J,L), GMN(J,L), XLMN(J,L), EEM(J,L), BUGP 410
2  BEEL(J,L), L=IY, J=1,9) BUGP 420
195 FORMAT (4H0IY=I3, 2X, HYY=IPE12.5, 2X, HIJ, 2X, HLM, 7X, 2HYD, 12X, 3HWMN, BUGP 430
1  12X, 3HGMM, 11X, 4HXLMN, 13X, 3HEEM, 13X, 3HBEY/(2I3, 6E16.5)) BUGP 440
  RETURN

50  WRITE (6,196) IY, YD(IY), ((J, L, YD(L), BUGP 500
1  WPP(J,L), GPP(J,L), XLPJ(J,L), EEP(J,L), BUGP 510
2  BEEL(J,L), L=IY, NES), J=1,9) BUGP 520
196 FORMAT (4H0IY=I3, 2X, HYY=IPE12.5, 2X, HIJ, 2X, HLM, 7X, 2HYD, 13X, 3HPPP, BUGP 490
1  2X, 3HGPJ, 11X, 4HXLPP, 13X, 3HEEP, 13X, 3HBEY/(2I3, 6E16.5)) BUGP 500
  RETURN

60  WRITE (6,198) IY, ETA(IY), YD(IY)
198 FORMAT (4H0IY=I3, 2X, 4HETA=IPE12.5, 2X, HYY=IPE12.5, 2X, HIJ, 5X, 3HMCC, BUGP 530
1  11X, 3HFP, 11X, 3HFC, 11X, 3HQLC, 11X, 3HQLS, 12X, 2HFPA, 12X, 2HFP, 12X, 2HFR/)
  WRITE (6,199) (J, QCCP(J), FMC(J,IY), FPC(J,IY),
2  QCLP(J), QLCP(J), QLIP(J), FM(J,IY), FP(J,IY),
2  J=1,9) BUGP 550
199 FORMAT (I3, 4PE14.5) BUGP 580
  WRITE (6,8069) (J, QCCP(J), FMC(J,IY), FPC(J,IY), J=10,12) BUGP 600
8069 FORMAT (I3, 4PE14.5) BUGP 610
  WRITE (6,200) QCC(IYY), QCL(IYY), QLCP(IYY), QLL(IYY),
1  DON(IYY) BUGP 630
200 FORMAT (1HO, 2X, 3PE14.5, 28X, 3E14.5, 28X, E14.5) BUGP 640
  RETURN

70  WRITE (6,197) L, ETA(L), YD(L), ((J, M, WN(J,M),
1  FG(J,M), GP(J,M), FMUL(J,L), TAUL(J,L),
2  SSM(J,M,L), GGJ(J,M,L), ETAM(J,M,L), SBM(J,M,L), BUGP 670
3  M=1,4), J=1,9) BUGP 690
197 FORMAT (3HOL=13, 2X, 4HETA=IPE12.5, 2X, 3HYD=E12.5, 2X, 1HJ, 2X, 1HM, 7X, BUGP 700
1 1HN*13X.1HF*13X.1HG*11X.3HFMU*11X.3HTAU*11X.3HSSM*11X.3HGGM*10X. BUGP 710
2 4HETAM*11X.3HSBM/((2\times3.9E14.5)) BUGP 720
RETURN BUGP 730
END BUGP 740
SUBROUTINE ZHV(HV,ZO,ZN,ZN,ZI,ZC)

** THIS SUBROUTINE CALCULATES THE QUANTUM MECHANICAL CORRECTION FACTORS GIVEN A FREQUENCY (HV) **

X = HV
X2 = X*X
X3 = X2*X
X4 = X3*X
X5 = X4*X
X6 = X5*X
X7 = X6*X

IF (X - 9.82) 1,1.2
1 Z0 = 6999795
   +6.677328 E-05*X3
   -3e6445e5 E-05*X4 +8.058070 E-04*XS
   +2.824548 E-02*X2
   ZHV( )
2 ZO = (X/9.82)**3
   ZHV( )
GO TO 3

3 IF (X - 8.35) 4,4.5
4 ZN = 1.000148
   -4183535 *X
   +3183535 *X2
   ZHV( )
1 ZN = 9.79458 E-02*X3
   +3.354635 E-02*X4 -5.609353 E-03*XS
   +4.515535-04*X6 -1.4035e5 E-05tX7
   ZHV( )
GO TO 8

8 ZI = 1.000379
   -4.2964767 *Y
   +7.505242 E-02*Y2
   ZHV( )
1 ZI = 1.702948E-02*Y3
   +3.279554 E-03*Y4 -2.128469 E-04*Y5
   ZHV( )
GO TO 11
10 ZI = (Y/6.6)**3
11 IF (X-7.e37) 12,12+13
12 ZC = .9974367 - .4341812 *X + 8.531314 E-02*X2
13 RETURN
END
14 RETURN
15 GO TO 14
16 ZC = (X/7.e37)**3
17 RETURN
18 END
Figure C.1 Temperature Profiles

Equilibrium (SLAC)

Non-Equilibrium (Balhoff)

Non-Equilibrium (SLAC)
Figure 6.2 Enthalpy Profiles
Figure C.3 Density Profiles
Figure C.4 Velocity Profiles
Figure C.5  Mass Fraction Profiles for C
Figure C.6  Mass Fraction Profiles for C₂
Equilibrium (SLAC)

Non-Equilibrium (Balhoff)

Non-Equilibrium (SLAC)

Figure 6.7  Mass Fraction Profiles for CO
Figure 5.8 Mass Fraction Profiles for $C_3$
Figure 6.9 Mass Fraction Profiles for C₃H
Figure 6.10: Mass Fraction Profiles for CN
Figure 6.34. Mass Fraction Profiles for $C_2H$
Figure C.12 Mass Fraction Profiles for C₄H
Figure C.13 Mass Fraction Profiles for HCN
Figure C.14 Mass Fraction Profiles for C$_2$H$_2$
Figure C.15 Mass Fraction Profiles for $C^+$
Figure C.76: Mass Fraction Profiles for N₂
Figure 6.17 Mass Fraction Profiles for N
Figure C. Mass Fraction Profiles for N⁺
Figure C. 19 Mass Fraction Profiles for O
Figure C.20 Mass Fraction Profiles for $O^+$

**In $C\bar{0}$**

**Non-Equilibrium (SLAC)**

**Non-Equilibrium (Balhoff)**

**Equilibrium (SLAC)**

*stagnation point*
Figure C.21 Mass Fraction Profiles for H₂
Figure C.22 Mass Fraction Profiles for H
Figure C.23 Mass Fraction Profiles for $e^-$
Guillermo Perez was born on [redacted]. He completed his secondary education at University High School, Rio Piedras, Puerto Rico in May, 1962. From August, 1962 until May, 1967 he attended the University of Puerto Rico at Mayaguez receiving the Bachelor of Science degree in Mechanical Engineering. In September 1967, following a brief period of employment at the Puerto Rico Water Resources Authority, he enrolled in the Graduate School of Louisiana State University, and in January 1970, he received the Master of Science degree in Mechanical Engineering. From February, 1970 until June 1972 Mr. Perez continued his studies towards the Doctor of Philosophy degree in Chemical Engineering at L.S.U. In July he went to work as Director of the Resource Management Division of Puerto Rico's Environment Quality Board (EQB). While working at the EQB Mr. Perez was subsequently named Director of the Water Quality Bureau (November 1972) and Technical Assistant to the Executive Director (March 1973). Since March 1974, he has been a partner in the consulting firm of Cummings, Perez & Co., a firm specializing in environmental planning. He intends to continue working towards the development of Cummings, Perez & Co.