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STAGNATION REGION HEATING OF A PHENOLIC-NYLON ABLATOR DURING RETURN FROM PLANETARY MISSIONS

by

Donald D. Esch, Research Associate

Ralph W. Pike, Co-principal Investigator

Carl D. Engel, Research Associate

Richard C. Farmer, Co-principal Investigator

John F. Balhoff, Research Associate

Department of Chemical Engineering

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LOUISIANA STATE UNIVERSITY

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by

Reacting Fluids Laboratory
Department of Chemical Engineering
Louisiana State University
Baton Rouge, Louisiana 70803

for

Langley Research Center
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

PREFACE

This report gives the results, in detail, for a stagnation-line analysis of the radiative heating of a phenolic-nylon ablator. The analysis includes flowfield coupling with the ablator surface, equilibrium chemistry, multicomponent or binary diffusion and a coupled line and continuum radiation calculation. This report serves as the documentation, i.e. users manual and operating instructions, for the computer programs listed in the report. Copies of the decks have been transferred to Mr. James N. Moss, grant monitor, of the Langley Research Center, and can be obtained from him or from the authors.

Due to the length of this report an abbreviated version giving the key information has been submitted to the Langley Research Center for reviewing and issuing as a NASA contractor's report. This report also served as the dissertation in chemical engineering for Donald D. Esch.

ACKNOWLEDGEMENTS

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The assistance of Mr. Dean Mayers, Mr. James Callender and Mr. Simon Hacker for special contributions to preparation of the report is gratefully acknowledged. The typing chores were very capably performed by Mrs. Elida Aronstein and Mrs. Carol Esch.

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ABSTRACT

A coupled numerical analysis of the radiative heating of ablative thermal protection systems was developed. The analysis includes flowfield coupling with the ablator surface, multicomponent diffusion, and a coupled line and continuum radiation calculation. With emphasis toward re-entry from planetary flight, the effects of assuming simplified transport and thermodynamic models were examined.

Comparisons were made in wall heating rate calculations assuming both binary and multicomponent diffusion. Further comparisons were made by performing heating rate analysis based upon the proper values of thermal conductivity and viscosity for the injected species and based upon using air properties for the injected species. Heat capacity was examined in a similar manner.

On the basis of this research, it was concluded that the binary diffusion assumption, as opposed to a rigorous multicomponent diffusion analysis, can yield accurate heating rate predictions provided the appropriate binary coefficient is employed. For low mass injection

rates, it was also observed that the choice of the binary coefficient was very critical in determining the correct wall heating rate.

For large blowing rates it was confirmed that the transport mechanisms (i.e., diffusion, conduction, and viscous transport) contribute very little ($\leq 5\%$) to the heat transfer process. Therefore, variations in property models are of little consequence. For low mass injection rates, thermal conductivity was observed to contribute significantly in determining heat transfer to the surface.

Heat capacity was found to be an important factor in determining temperature distributions throughout the flowfield. In the presence of high radiative heating, large differences in the temperature distributions were observed when the simplified (air) property was used instead of the appropriate value.

In comparison with the performance of carbon-phenolic ablators, the 40% nylon-60% phenolic resin ablator was observed to be approximately 5% less effective in blocking radiation to the ablator surface.

CHAPTER I

INTRODUCTION AND BACKGROUND

Introduction

It is the purpose of this research to quantitatively establish the effects of several assumptions used in the prediction of gas-dynamic heating of re-entry vehicles. Particular emphasis will be given to analyses at flight conditions characteristic of re-entry from planetary missions. This chapter will serve as a general introduction to the subject of re-entry heating and will establish the appropriate groundwork for analytical development in subsequent chapters.

The chapter will consist of three parts with the first being a brief overview of aerodynamic heating and thermal protection systems, specifically the charring ablator. This discussion will then be followed by an evaluation of the importance of, and difficulties associated with, accurate heating rate calculations for future manned and unmanned planetary missions. The chapter will be concluded with a specific statement of objectives for the current study.

Aerodynamic Heating

If a body entering a planetary atmosphere utilizes aerodynamic drag to reduce its speed for a soft landing, all of the kinetic energy possessed by the vehicle at entry must be converted to heat. As shown in Figure 1.1, this quantity of energy can be very large (10^3-10^5 BTU/lb). This figure also demonstrates the relative advantage of ablative materials over heat sinks as thermal protection systems (Ref. 1.1).

The heating rates suggested by Figure 1.1 are somewhat misleading since, as will be demonstrated, it is not necessary for the energy equivalent to the total kinetic energy to reach the surface of the vehicle. It can be shown that the total heat input for re-entry can be approximated by the following relationship (Ref. 1.1):

$$H = \frac{c_h}{c_d}\left(1/2\ mU_\infty^2\right) = \frac{c_f}{2c_d}\left(1/2\ mU_\infty^2\right) \qquad (1.1)$$

where

H = total heat input to the vehicle

m = vehicle mass

U_∞ = entry velocity

c_h = heat-transfer coefficient

c_d = drag coefficient

c_f = friction coefficient

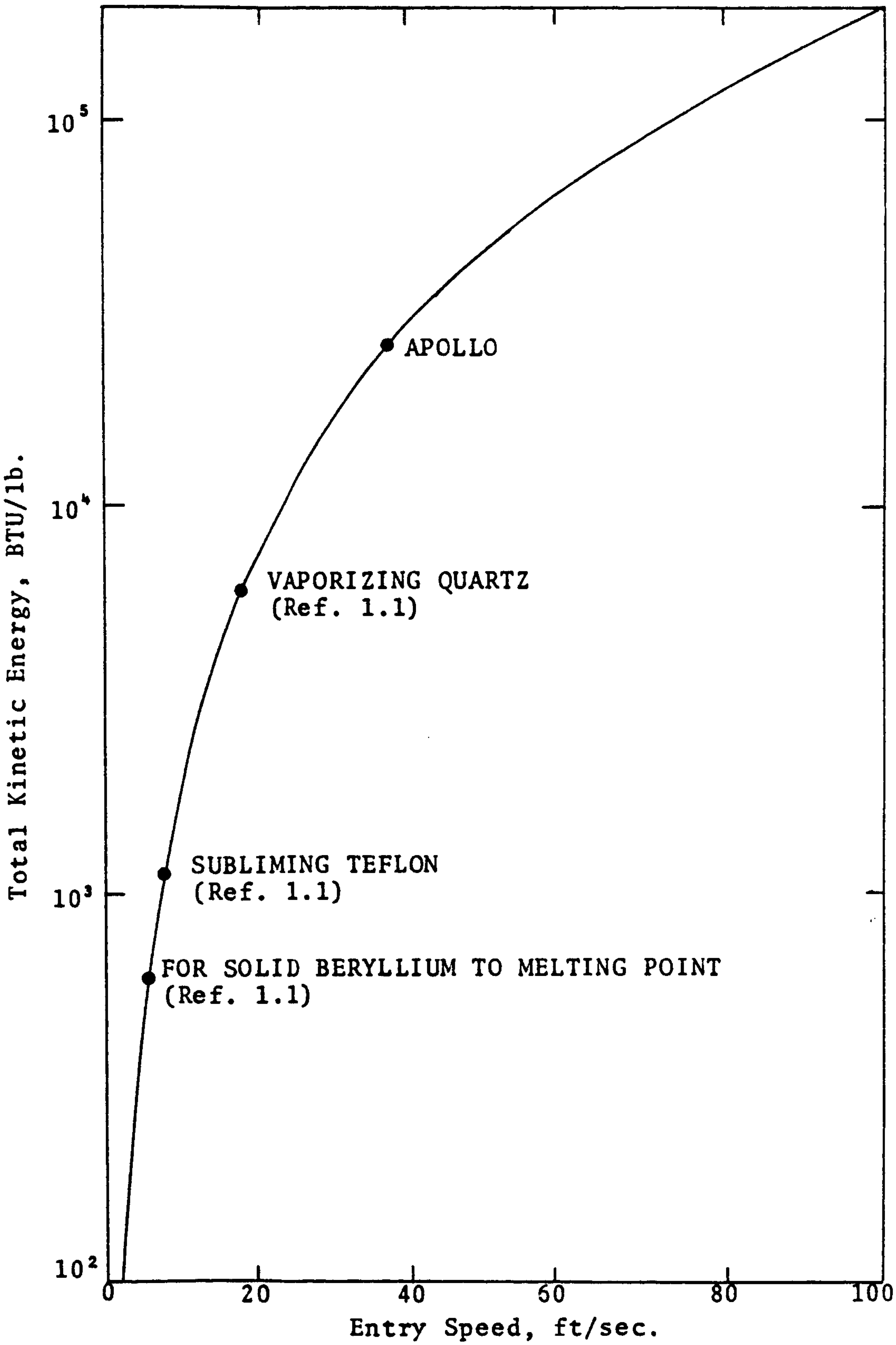


Figure 1.1. Total Kinetic Energy of a Body in Motion.

For blunt bodies (i.e., those having high drag coefficients), the ratio of the heat-transfer coefficient to the drag coefficient is less than for streamline bodies under the same conditions. A typical value for this ratio of coefficients for hypersonic flow over a blunt body is 0.005, assuming laminar boundary layer (Ref. 1.1).

In spite of the reduction in total heating achieved by using blunt bodies for re-entry vehicles, the relative amount of heat absorbed by the vehicle is still sufficient to produce surface temperatures in excess of 3000°K. Thus highly efficient thermal protection systems are required. As previously noted in Figure 1.1 the ablative thermal protection system is more effective than simple heat sinks since large amounts of energy are absorbed by the phase and chemical changes that occur.

Charring Ablators

A wide range of ablative materials have been investigated extensively for use as thermal protection systems for high speed Earth entry and planetary atmospheric flight. A selected list of these investigations is reported in Reference 1.2. As a result of these studies it was found that charring ablators, such as reinforced plastics and castable epoxy resins, provide a relatively efficient heat protection system with a wide range of versatility (Ref. 1.2). Currently, the technology associated with charring ablators is quite well established as the result of numerous analytical and experimental studies over the last decade; for example, see References 1.3 to 1.10. Considering the advanced technology of charring ablators, this thermal protection system is currently most desirable for the early manned planetary missions.

An illustration of the process of charring ablation is given in Figure 1.2. The ablation process and accompanying flow-field interaction occurs as follows: the virgin plastic, e.g., virgin, phenolic resin-nylon composite, is heated by conduction to its decomposition temperature (approximately 1000°K), where endothermic cracking of the polymer occurs, producing hydrocarbon gases which pass outward through the porous, charred remains of previously decomposed plastic. The pyrolysis products are then expelled into the boundary layer adjacent to the charred surface, carrying with them an additional quantity of carbon gas provided by the subliming char interface. Thus at equilibrium, the surface temperature of the gas-solid interface is approximately equal to the sublimation temperature of the solid (~3450°K for carbon).

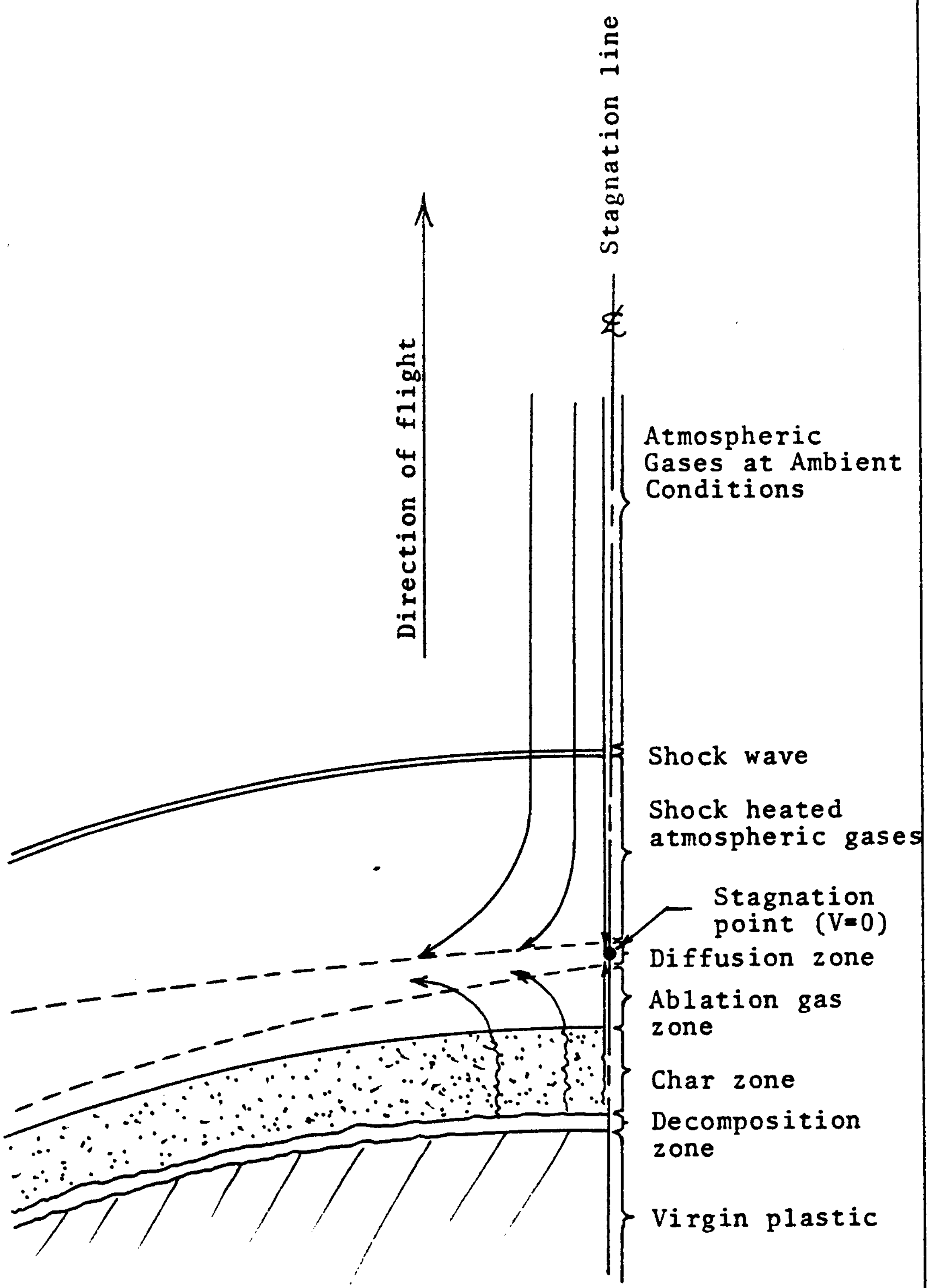


Figure 1.2. Illustration of Charring-Ablator and Flowfield Interaction.

At the outer edge of the boundary layer, shock heated atmospheric gases ($\sim 15{,}000^{\circ}K$) move primarily by convection toward the stagnation point, where the diffusive mechanism becomes predominant. The region in the immediate vicinity of the stagnation point is thus indicated in Figure 1.2, as a diffusion zone.

Although simply depicted in Figure 1.2, the overall process is quite complex and presents a significant challenge to an accurate mathematical analysis. The major difficulty arises in determining the net radiative heating incident upon the ablating surface. In Figure 1.3, the primary heat transfer mechanisms associated with this problem are illustrated. The discussion to follow will consist of an elementary description of these mechanisms.

In the shock-heated, atmospheric gas region, while radiative absorption does occur, the predominant radiation effect is emission, which naturally occurs in all directions. Precursor heating arises when the radiative flux through the shock is absorbed by the ambient gases thus increasing the free-stream enthalpy and resulting in even higher temperatures subsequent to the shock heating. The radiative flux in the direction of the body is partially absorbed in the ablation layer, increasing the temperature of the gases in the region; the

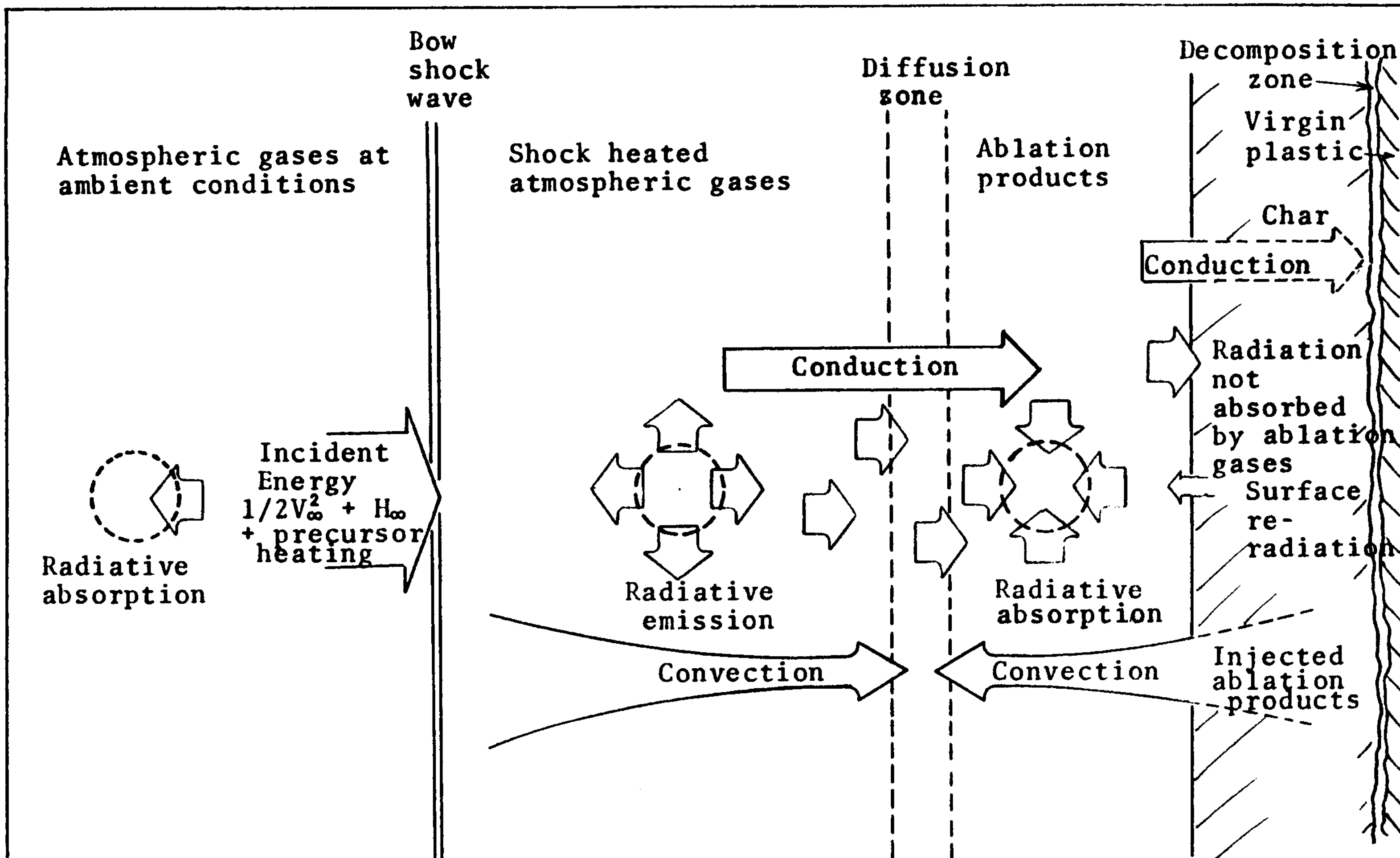


Figure 1.3. Illustration of Heat Transfer Mechanisms in Ablating Thermal Protection Systems.

remaining energy is absorbed by the solid interface to be re-radiated or transported by conduction through the char into the decomposition zone. In the ablator the energy is absorbed by the endothermic reactions of the pyrolysis gases in the char zone and the decomposition of the polymer. The small fraction of energy not assimilated in the char and decomposition zones is finally absorbed by conduction into the virgin plastic.

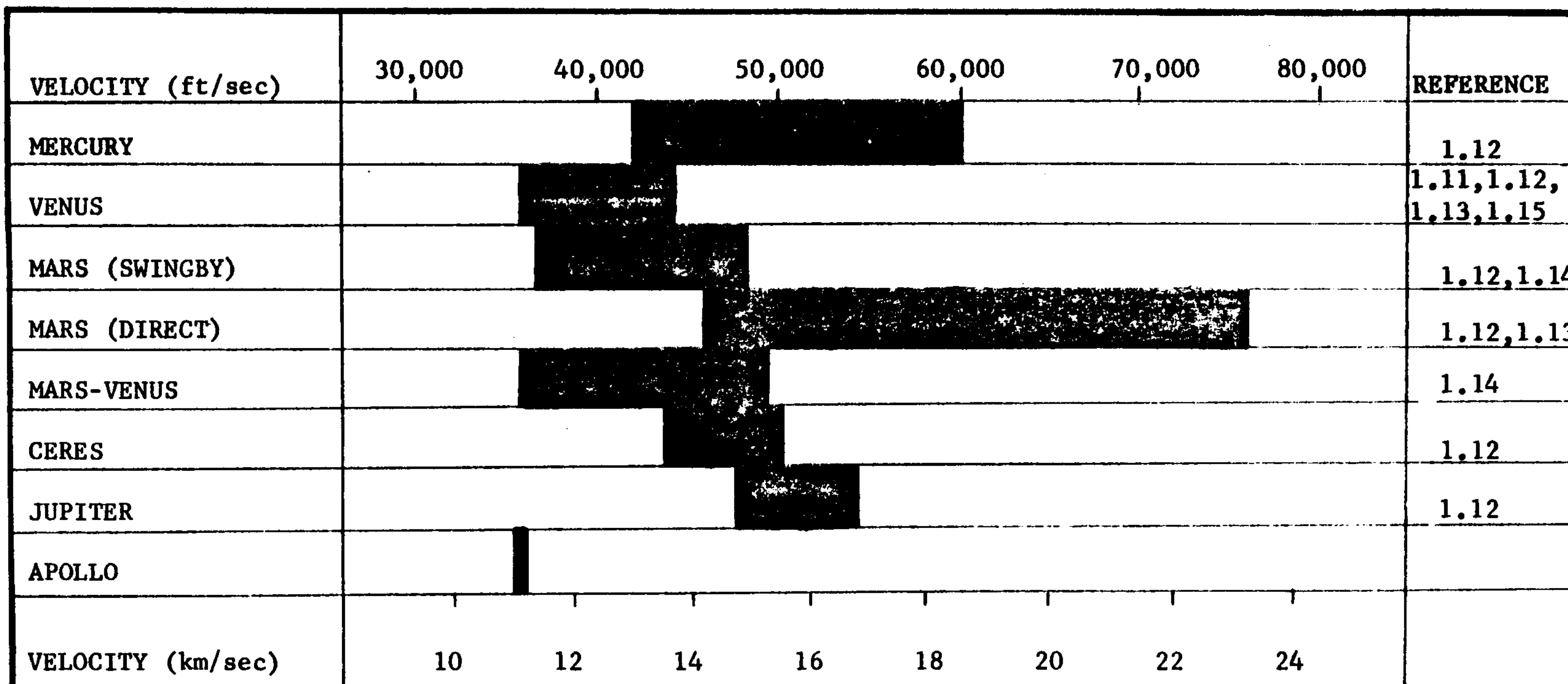
The preceding description clearly shows the intimate coupling between the response of the thermal protection system and the radiation heat transfer process. Since radiative transport is determined by the temperature and composition of the system, it stands to reason that any approximation used in the evaluation of these dependent variables would be reflected in the radiation calculation and thus the ablator response. Correspondingly, more rigorous calculations could substantially alter the prediction of flowfield characteristics and the surface heating rates.

The Importance of Accurate Radiative Heating Rate Predictions

The current uncertainty in radiative heating rate predictions at entry velocities characteristic of lunar return is minimal compared to other uncertainties in predicting heat shield performance at this flight condition. Consequently refinements in these calculations would yield relatively small increases in accuracy. However, for those velocities anticipated for planetary entry and return, radiative heating is expected to play a far more important role (See Table 1.1). An estimate of the increase in radiative and convective heating for increasing entry velocity is shown in Figure 1.4. As a result of the dramatic increase in radiation heating, many of the currently acceptable assumptions in heating rate calculations may becomes intolerable, particularly those assumptions which relate to the prediction of species compositions. One such assumption is that of local chemical equilibrium as opposed to finite-rate chemistry. Another is the assumption of binary diffusion (Fick's Law) versus a multicomponent diffusion analysis. Others include--simplifications in transport properties, such as using air properties throughout the flowfield and neglecting thermal diffusion; simplified radiation models; and the assumption of a laminar flowfield. In Figure 1.5, the uncertainties in heat shield weight requirements are estimated for the approximate range of entry velocities anticipated in future planetary missions. According to

Table 1.1

Expected Earth Entry Velocities for Several Planetary Missions



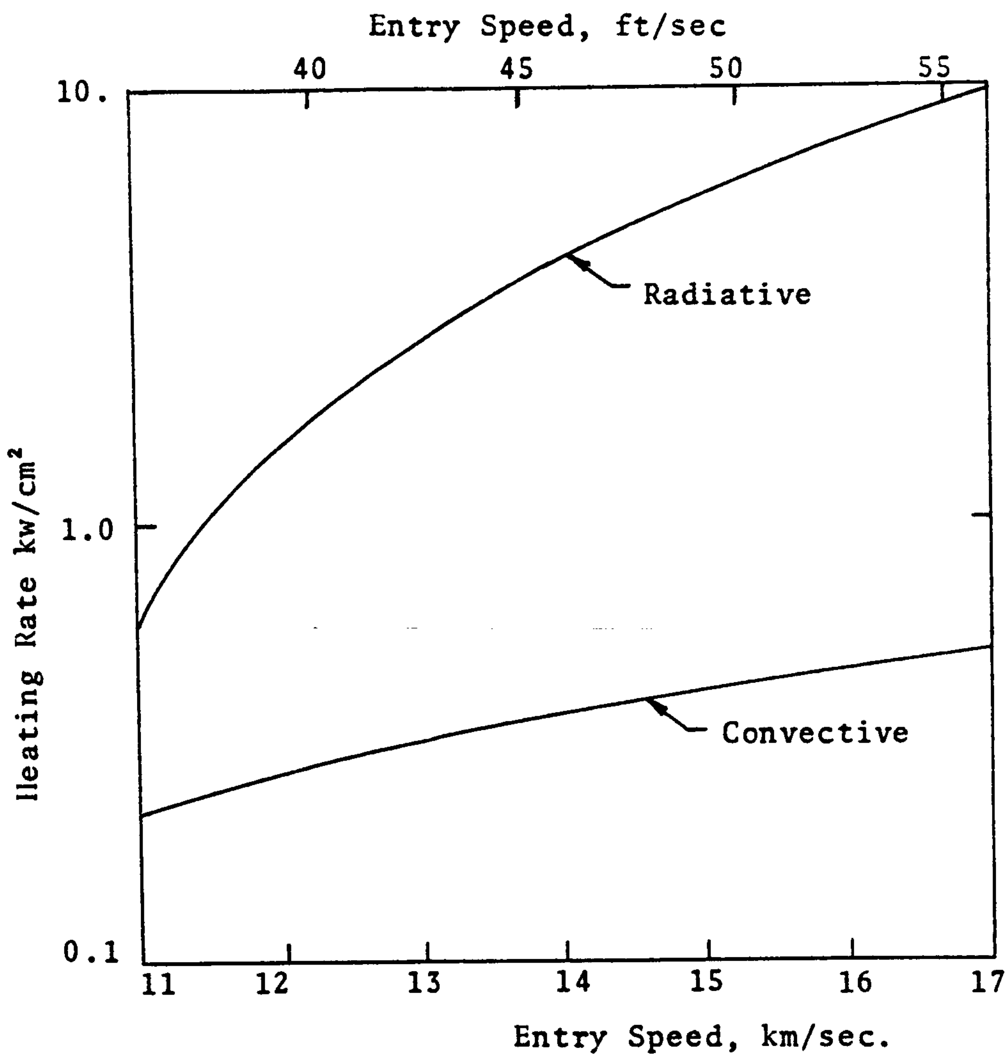


Figure 1.4. Peak Stagnation Point Heating Rates; Blunt Body, L/D = 0.5 (Ref. 1.12).

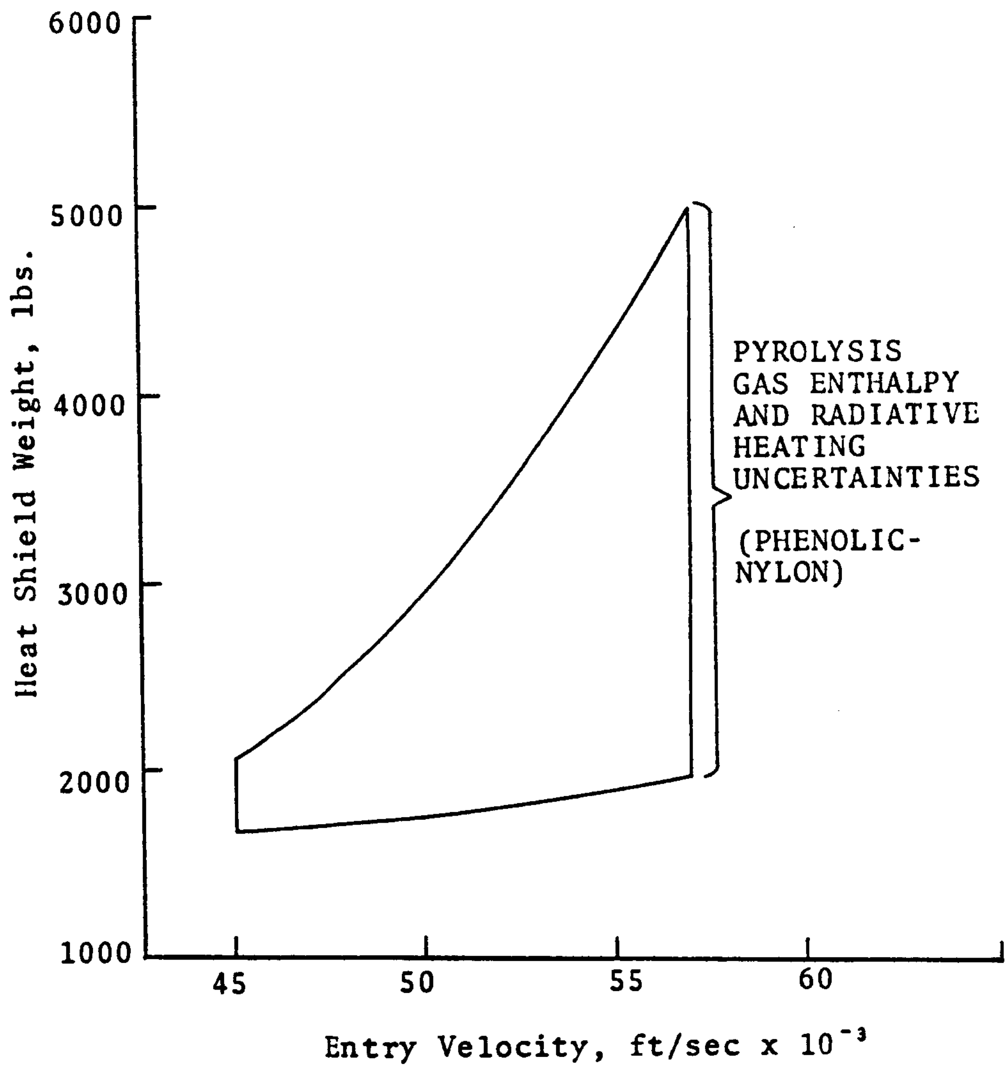


Figure 1.5. Weight Sensitivity for Planetary Return (Eight Man Crew, Ref. 1.11).

one estimate, each pound carried throughout a manned planetary mission can represent between 300 and 1000 pounds on the launch pad (Ref. 1.12). Assume that each pound of heat shield only represents 300 pounds of launch pad weight. Using Figure 1.5 an uncertainty of 180 tons in the weight of the launch vehicle would then exist for an entry velocity of 50,000 feet per second.

Statement of Objectives

In an effort to reduce uncertainties such as those previously illustrated, the current research was undertaken. Specifically, the current study will include the assessment of two important effects:

1. The effect upon radiation heating of the more accurate multicomponent diffusion analysis versus simple Fickian diffusion.

2. An evaluation of the effect upon radiant heating of using appropraite transport and thermodynamic properties, as opposed to the simplification of using air properties throughout the flowfield.

The flight conditions selected for these comparisons will be characteristic of those anticipated for re-entry from planetary missions.

Subsequent studies will be aimed at resolving additional uncertainties in current analyses by including finite-rate chemistry, by performing a thorough assessment of radiation properties, and including these results in a fully coupled analysis of the ablator-flowfield interaction. The overall goal of all of the studies will be to develop an optimum model for use in thermal protection system design calculations where radiant heating is the dominant heat transfer mechanism.

The following chapter will consist of a detailed review of previous literature on multicomponent diffusion studies and of pertinent investigations in the prediction of high temperature transport and thermodynamic properties. In addition, a review and comparison of previous investigations of radiation coupled heating rate analyses will be presented.

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CHAPTER II

A REVIEW OF PREVIOUS ANALYSES IN MULTICOMPONENT REACTING GAS SYSTEMS

Historical Development of Dilute-Gas Transport Equations

An excellent historical summary of the early development of the hydrodynamic transport equations is given in Chapman and Cowling (Ref. 2.1). The formulation and development had its origins in a classic paper by J. C. Maxwell, in 1867 (Ref. 2.2). His paper, "On the Dynamical Theory of Gases", contains a derivation of the general equations of transfer describing the total rate of change of any mean property. The solution to these relationships required the specification of a molecular velocity distribution function. To obtain a solution, Maxwell, thus proposed the distribution function which is given his name today. Boltzmann, in 1872 (Ref. 2.3) gave his famous integro-differential equation* which the velocity distribution function must satisfy. From the Boltzmann equation, the equations of change (the equations of conservation of mass, momentum

*See Ref. 2.8, p. 452, Equation 7.1-25.

and energy) could theoretically be derived without having specified the velocity distribution function. Assuming a Maxwellian distribution, Boltzmann confirmed the equations proposed by Maxwell; however, he was never able to obtain a satisfactory solution to his own equation.

> He gave a complicated approximate method of solution with the object of calculating viscosity. The investigation, which in all occupies 168 pages of his Collected Works, appeared to yield no simple result, and Boltzmann remarked that one must despair of the general solution of his equation. (Ref. 2.1)

Nearly a half a century later the general solution was finally realized. Independently, solutions were derived by Chapman (Ref. 2.4) in 1916 and Enskog (Ref. 2.5) in 1917. With the exception of minor theoretical revisions, their solution to the Boltzmann equation has remained unchanged during the past four decades. Hence the name, "Chapman-Enskog Theory", has come to mean the rigorous kinetic theory of dilute (low pressure) monatomic gas mixtures. Accordingly, the "Chapman-Enskog" equations are those describing the transport coefficients (viscosity, thermal conductivity, and diffusion coefficients) of dilute gases. With a few modifications to account for the presence of polyatomic molecules, these equations will serve as a basis for the current analyses.

For the most part, the remainder of this chapter will be devoted specifically to a review of one aspect of dilute gas transport phenomena, the diffusion of chemical species in reacting gas mixtures. In the course of surveying this topic, it will be necessary to include a discussion of the various formulations and nomenclature commonly employed in gaseous diffusion calculations, for example: the Stefan-Maxwell equations; multicomponent, binary and effective diffusion coefficients; and frames of reference. Following the survey of multicomponent diffusion studies, the chapter will be concluded with a review of current radiation-coupled analyses of ablating thermal protection systems and a summary of the results of previous studies into the effects of transport property variations upon heating rate predictions.

Diffusion in Dilute Multicomponent Gases

Multicomponent Diffusion Coefficients: Through solutions of the Boltzmann equation, Hellund (Ref. 2.6) and later Curtiss and Hirschfelder (Ref. 2.7) obtained theoretical formulations describing the diffusive behavior of a mixture of several gases. The equation describing the diffusive mass flux vector (J_i) of the ith species relative to the mass average velocity ($\overline{v}$) is given in Hirschfelder, Curtiss, and Bird (Ref. 2.8, p. 516). The flux vector (neglecting pressure diffusion and forced diffusion) is written as,*

$$J_i = \frac{n^2}{\rho} \sum_{j=1}^{\nu} m_i m_j D_{ij} \, \nabla Y_j - D_i^T \, \nabla \ln T$$

$$i=1,\ 2,\ldots,\nu \qquad (2.1)$$

where $J_i = \rho_i \overline{V}_i = \rho_i \ (\overline{v}_i - \overline{v})$ (2.2)

The D_{ij}'s appearing in Equation 2.1 are referred to as multicomponent diffusion coefficients. These are not to be confused with the binary diffusion coefficients, $\mathcal{D}_{ij}$, which are computed directly from molecular properties by the following Chapman-Enskog equation:

$$\mathcal{D}_{ij} = 2.28 \times 10^{-7} T^{3/2} \left(\frac{M_i + M_j}{2 M_i M_j}\right)^{1/2} / \ p \sigma_{ij} \Omega_{ij}^{(1,1)} \ \text{ft}^2/\text{sec}$$

(2.3)

From the composition and the binary diffusion coefficients, the multicomponent diffusion coefficients can be determined by means of the matrix formulation given in Hirschfelder, Curtiss, and Bird (Ref. 2.8, p. 541). The

*For specific definition of terms, the reader is referred to the nomenclature section.

same reference gives a similar formulation from which the thermal diffusion coefficients, D_i^T, can be computed (p. 543).

For most calculations, the effects of pressure, forced and thermal diffusion can be neglected and, Equation 2.1 can be expressed as follows:

$$J_i = \frac{\rho}{M} \sum_{j=1}^{n} M_i M_j D_{ij} \nabla Y_j \qquad i=1, 2, \ldots, \nu \qquad (2.4)$$

Because of the concentration dependence of the multicomponent diffusion coefficients, this type of formulation is inconvenient to use (Ref. 2.9). For this reason various modifications of the previous form are frequently more desirable for computational purposes. In Reference 2.7, Curtiss and Hirschfelder demonstrated that for an ideal gas mixture, Equation 2.1 (or Equation 2.4) could be rearranged into a form which is expressed entirely in terms of the binary diffusion coefficients. This form is referred to as the Stefan-Maxwell Equations.*

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*Maxwell's contribution to the development of the transport equations has been discussed earlier in this chapter. The inclusion of Stefan's name in the title of the equations is most likely based upon his being the first to specifically examine the diffusion aspect of transport equations (Ref. 2.12).

<u>The Stefan-Maxwell Equations</u>. The most frequently used approach to the solution of multicomponent, gas-diffusion problems involves the use of the Maxwell or Stefan-Maxwell Equations. A derivation of these relations from Equation 2.1 is given in Reference 2.8 (p. 485). In the absence of the thermal diffusion, forced and pressure diffusion, the equations are written as follows (Ref. 2.9, p. 570):

$$\nabla Y_i = \sum_{j=1}^{\nu} \frac{Y_i Y_j}{\mathcal{D}_{ij}} \quad (V_j - V_i) \qquad i=1, 2, \ldots, \nu \quad (2.5)$$

In matrix form these equations can be conveniently represented in the following way for one coordinate direction

$$\bar{\bar{A}}\, V_y = \frac{\partial \bar{Y}}{\partial y} \qquad (2.6)$$

where the coefficients a_{ik} are,

$$a_{ik} = \frac{Y_i Y_k}{ik} \quad (i \neq k) \qquad (2.7)$$

$$a_{ii} = - Y_i \sum_{j \neq i} \frac{Y_j}{\mathcal{D}_{ij}} \qquad (2.8)$$

and V_y is the vector of diffusion velocities of the ν species in the y direction.

The system given by Equations 2.5 or 2.6 is not linearly independent as discussed in Reference 2.11. In fact, there are only ν-1 linearly independent equations. The physical meaning of this occurence arises from the fact that the diffusion velocities, V_i, are relative to the mixture flow velocity as defined in Equation 2.2. It is therefore necessary to establish some frame of reference, which can be applied to obtain an independent set of equations.

Reference Frames in Diffusion. The specification of the required reference frame is equivalent to defining the mixture flow velocity. Definitions of mixture flow velocity which are commonly employed are the local mass average velocity, molar average velocity or the volume average velocity, the choice being based upon the convenience of formulation. Several good discussions concerning the choice of these and other reference frames are available throughout the literature (Refs. 2.9-2.11). In this study, the mixture flow velocity is defined as the local mass average velocity:

$$\overline{v} = \sum_{i=1}^{\nu} \rho_i \overline{v}_i / \sum_{i=1}^{\nu} \rho_i \qquad (2.9)$$

where $\overline{v}_i$ is the velocity of the ith species with respect to stationary coordinate axis. As previously stated, the diffusion velocities, $\overline{V}_i$ appearing in Equation 2.6 are expressed relative to the mixture flow velocity.

$$\overline{V}_i = (\overline{v}_i - \overline{v}) \tag{2.10}$$

From this relationship and the assumed frame of reference, the local mass average velocity, the sum of the mass fluxes over all species can be determined:

$$\sum_{i=1}^{\nu} \rho_i \overline{V}_i = \sum_{i=1}^{\nu} \rho_i \overline{v}_i - \overline{v} \sum_{i=1}^{\nu} \rho_i \tag{2.11}$$

From Equation 2.9,

$$\sum_{i=1}^{\nu} \rho_i \overline{v}_i = \overline{v} \sum_{i=1}^{\nu} \rho_i \tag{2.12}$$

therefore

$$\sum \rho_i \overline{V}_i = 0 \tag{2.13}$$

Since this relationship between mass fluxes is based upon the selected frame of reference, it provides the necessary condition for completely defining the diffusion velocities, $\bar{V}_i$. By replacing one of Equations 2.5 by Equation 2.13, the diffusion velocities can be determined. Analogous developments can be performed for various other reference frames.*

Common Diffusion Coefficients. For a binary system of components A and B, Equation 2.4 simplifies to Fick's law such that,

$$\bar{J}_A = - \rho/M^2 \quad M_A M_B \mathcal{D}_{AB} \frac{\bar{\nabla} Y_A}{dy} \tag{2.14}$$

$$\bar{J}_B = - \rho/M^2 \quad M_A M_B \mathcal{D}_{BA} \frac{\bar{\nabla} Y_A}{dy} \tag{2.15}$$

When expressed in terms of mass fractions rather than mole fractions, these equations become,

$$\bar{J}_A = - \rho \mathcal{D}_{AB} \bar{\nabla} C_A \tag{2.16}$$

$$\bar{J}_B = - \rho \mathcal{D}_{BA} \bar{\nabla} C_B \tag{2.17}$$

Upon examining the Chapman-Enskog equations from which the binary diffusion coefficients are computed (Equation 2.3) it is seen that the coefficients $\mathcal{D}_{AB}$ and $\mathcal{D}_{BA}$ are equal. Thus the diffusive behavior of binary system can

*A discussion of several other frames of reference is given in Reference 2.11.

be determined from the specification of a single coefficient. In an effort to extend this simplification to multicomponent systems, several authors (Refs. 2.13-2.17) have replaced the exact expression for mass flux in multicomponent mixtures (Equation 2.4) by Fick's Law,

$$J_i = - \rho D \nabla C_i \qquad i=1, 2, \ldots, \nu \tag{2.18}$$

The selection of the appropriate diffusion coefficient usually is satisfactory as long as the mixture is composed of similar species. However, for systems containing very dissimilar molecules, no basis exists for estimating a characteristic diffusion coefficient (Ref. 2.27). In the subsequent discussions, the use of the formulation given in Equation 2.18 will be referred as the "binary diffusion approximation."

Effective Diffusion Coefficients. When using the terminology, "effective diffusion coefficients", a distinction must be made between the approximate coefficients obtained from the derivation of Wilke (Ref. 2.18) and those obtained from the exact formulation employed by Tirskii (Refs. 2.19-2.21). The Wilke equation, given below, is derived from the Stefan-Maxwell equations assuming the diffusion of one component, A, into a stagnant mixture of gases, B, C, D . . . The equation, which is exact only under the above conditions is,*

$$D_A = \frac{1 - Y_A}{\frac{Y_B}{\mathcal{D}_{AB}} + \frac{Y_C}{\mathcal{D}_{AC}} + \frac{Y_D}{\mathcal{D}_{AD}} + \ldots} \tag{2.19}$$

The effective diffusion coefficient referred to by Tirskii is not limited by the previous assumption and is obtained in the following manner:

Assume a Fickian-like diffusion where

$$J_{i,y} = J_i = -\rho D_i \frac{\partial C_i}{\partial y} \tag{2.20}$$

In terms of mass concentrations, the Stefan-Maxwell equations can be written in one dimensional form as shown below:

$$\frac{\partial C_i}{\partial y} = \frac{M}{\rho}\left[\sum_j \frac{C_i J_j - C_j J_i}{\mathcal{D}_{ij} M_j} - C_i \sum_k \sum_j \frac{C_k J_j - C_j J_k}{\mathcal{D}_{kj} M_j}\right] \tag{2.21}$$

By combining Equations 2.20 and 2.21 an exact relationship for the effective coefficient, D_i, is thus obtained.

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*Excellent agreement was found in the experimental verification of this equation (Refs. 2.18 and 2.22). These results are an encouraging indication of the validity of the Stefan-Maxwell equations.

$$\frac{1}{D_i} = \frac{M}{J_i}\left[C_i \sum_k \sum_j \frac{C_k J_j - C_j J_k}{\mathcal{D}_{kj} M_j} - \sum_j \frac{C_i J_j - C_j J_i}{\mathcal{D}_{ij} M_j}\right] \tag{2.22}$$

Such a relationship as Equation 2.22 is best suited for an iterative numerical solution such as that proposed in Tirskii's latter paper (Ref. 2.21) and as that employed in this study.*

The Bifurication Approximation. In Reference 2.23, Bird demonstrated that a bifurication (separation) of the effects of the interaction between species permits an explicit solution to the Stefan-Maxwell equations for the mass fluxes. The empirical approximation used for this simplification was

$$\mathcal{D}_{ij} \simeq \bar{D}/F_i F_j \tag{2.23}$$

where $\bar{D}$ is an arbitrary reference diffusion coefficient and the parameters, F_i and F_j, are diffusion factors for species i and j.**

Using Equation 2.23, the explicit solution can be developed as shown in Reference 2.25 (Appendix B). The result is expressed as:

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*Presented in Chapter V.

**A method for computing these parameters is described in Reference 2.25 (Appendix C).

$$J_{i,y} = -\frac{\rho \bar{D}}{\psi_1} \left[\frac{\psi 2}{M} \frac{\partial z_i}{\partial y} + \frac{(z_i - C_i)}{M} \frac{\partial \psi 2}{\partial y} \right.$$

$$\left. + C_i \left(\frac{1}{F_i^2} \frac{dF_i}{dT} - \psi_4 \right) \frac{\partial T}{\partial y} \right] \tag{2.24}$$

where,

$$z_i = M_i Y_i / F_i \psi_2 = MC_i / F_i \psi_2 \tag{2.25}$$

$$\psi_1 = \sum_j Y_j F_j = M \sum_j C_j F_j / M_j \tag{2.26}$$

$$\psi_2 = \sum_j M_j Y_j / F_j = M \sum_j C_j / F_j \tag{2.27}$$

$$\psi_4 = \sum_j (C_j / F_j^2) \frac{\partial F}{\partial T} \tag{2.28}$$

It has been found that it is often consistent with the level of approximation to consider F_i independent of temperature (Refs. 2.24 and 2.26) Equation 2.24 is thus simplified to the following form:

$$J_{i,y} = -\rho \frac{\bar{D}\psi 2}{\psi_1 M} \left[\frac{\partial z_i}{\partial y} + \left(\frac{z_i - C_i}{\psi_2} \right) \frac{\partial \psi 2}{\partial y} \right] \tag{2.29}$$

The accuracy of the foregoing approximation to multicomponent mass fluxes has been investigated by Bartlett and Grose (Ref. 2.28) and Graves (Ref. 2.29). The former study involved a coupled ablator-flowfield analysis in which the use of the bifurication approximation gave predictions of mass injection rates which agreed within 5.0% of those predicted using an exact method. The investigation by Graves gave results which were quite favorable of the bifurication model. It was reported that in general there was little detectable difference between the multicomponent and the bifurication diffusion models. More discussion of the latter analysis will be included in a later development.

In the following section, the review of multicomponent diffusion analyses will be extended by examining the results of some analytical solutions. From these studies, certain phenomena are found to occur which might not be predicted by some of the previously discussed approximate methods.

Analytical Studies of Diffusion

Cross-effects Unique to Multicomponent Analyses: Several specific solutions to the Stefan-Maxwell equations have been reported in the literature (for example, Refs. 2.30-2.36). Although these solutions are all limited to tertiary systems, some anomalies unique to multicomponent diffusion are revealed. From the previously discussed multicomponent formulations, Equations 2.1 and 2.5, it is observed that the diffusive behavior of each component is not simply a function of its own gradient as is the case with binary diffusion. Instead, an additional dependency upon the gradients of the other components is seen to exist. As reported in the analytical investigation of Toor (Ref. 2.35), this occurrence gives rise to the following phenomena:

> Under certain conditions there exists,
>
> (1) a "diffusion barrier" such that the rate of diffusion of a component is zero even though its own concentration gradient is finite.
>
> (2) a condition, "osmotic diffusion," under which diffusion of a component may occur in spite of its own gradient being zero.
>
> (3) "reverse diffusion," when a component diffuses against its own gradient.

In Figure 2.1, an analytical solution to the Stefan-Maxwell equations for a tertiary system consisting of CO_2, H_2O, and H_2, are shown to demonstrate these occurrences. If effective diffusion coefficients were employed, a negative effective coefficient would

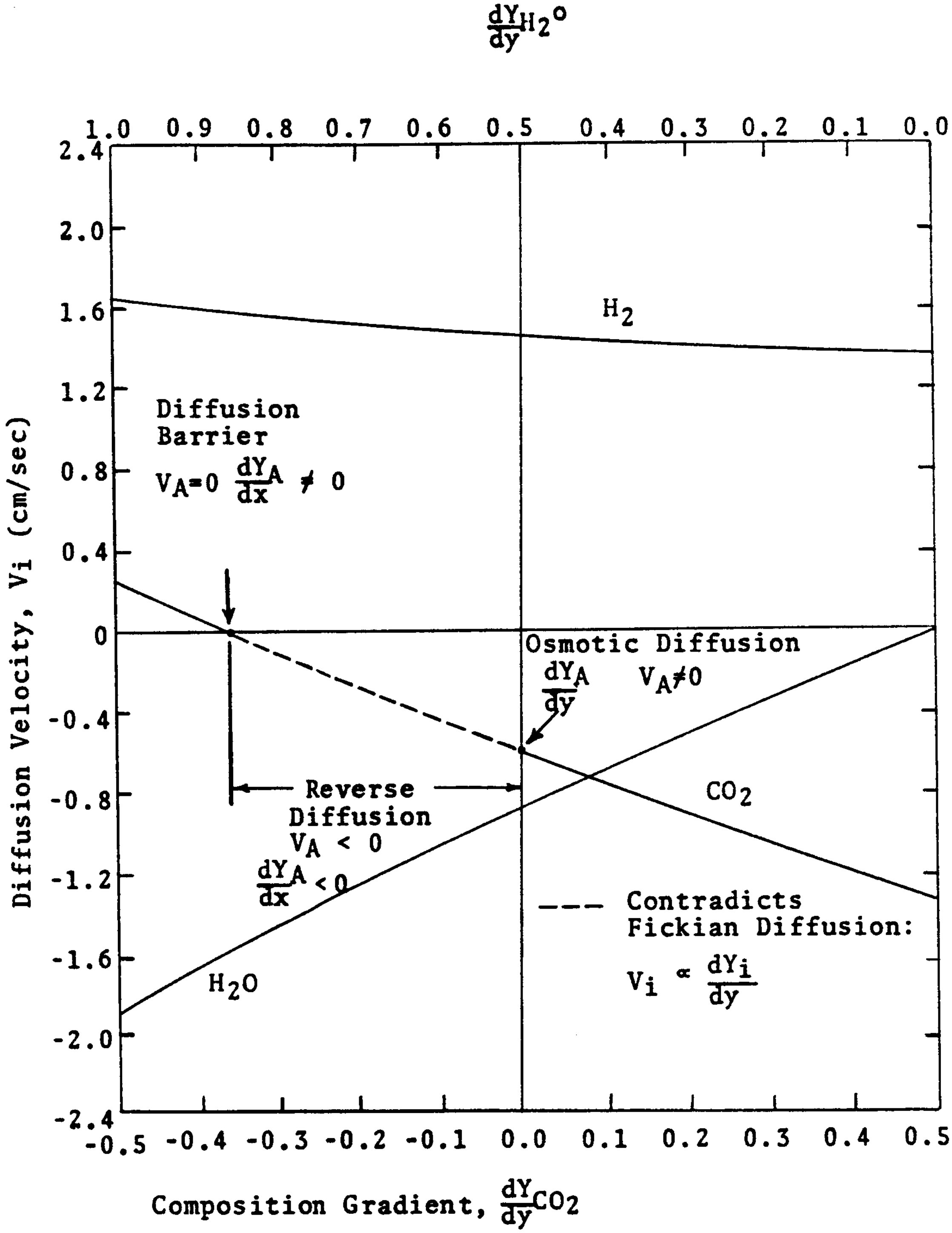

Figure 2.1. Diffusion Velocities as a Function of Mole Fraction Gradient (Ref. 2.35).

appear for CO_2 in the reverse diffusion region while the other coefficients would be positive. Since the binary diffusion approximation requires a common coefficient for all species, it is quite obvious that such an assumption is in contradiction to multicomponent behavior when reverse diffusion occurs.

<u>Linearization of Diffusion Formulation</u>. In recent papers by Toor (Ref. 2.37) and Cullinan (Ref. 2.38) it has been demonstrated that the species equations with mass fluxes expressed inthe form of Equation 2.1, can be transformed in such a way that the equations become uncoupled in the diffusion terms. In matrix form, Equation 2.1 can be written:

$$\bar{J}_y = \frac{\rho}{M^2} \bar{\bar{\mathbb{D}}} \frac{\partial \bar{Y}}{\partial y} \tag{2.30}$$

where

$$\mathbb{D}_{ij} = M_i M_j D_{ij}$$

Toor and Cullihan demonstrated that a non-singular matrix, $\bar{\bar{T}}$, exists, such that $\bar{\mathbb{D}}$ reduces to a diagonal matrix by the following transformation:

$$\bar{\bar{T}}^{-1}\,\bar{\bar{D}}\,\bar{\bar{T}} = \begin{bmatrix} \tilde{D}_{11} & & \bigcirc \\ & \ddots & \\ \bigcirc & & \tilde{D}_{\nu\nu} \end{bmatrix} \tag{2.31}$$

In this way the diffusion terms of the species equations can be decoupled by assuming that $\tilde{D}_{ii}$ is concentration independent. The latter assumption severely restricts the use of the Toor-Cullinan transformation to systems where concentration differences are relatively small.

Previous Analyses of Ablating Thermal Protection Systems With Radiation Coupling

There are four research groups that have reported stagnation line analyses which include mass injection of ablation products with radiation coupling. These investigators are: Rigdon, Dirling, and Thomas of the McDonnell Douglas Corporation (Refs. 2.15 and 2.48); Hoshizaki, Wilson, and Lasher of Lockheed Missiles and Space Company (Refs. 2.16, 2.49, and 2.50); Smith, Suttles, Sullivan, and Graves at NASA Langley Research Center (Ref. 2.14); and Chin, also at Lockheed (Ref. 2.51).

Rigdon, Dirling, and Thomas derived from the thin shock equations and subsequently solved the following viscous, stagnation-line, equations over the entire flowfield. The equation set solved was:

Continuity and X-Momentum:

$$\frac{d}{dy}\left(\mu \frac{d}{dy} \quad \frac{1}{\rho} \frac{d(\rho v)}{dy}\right) - \rho v \frac{d}{dy} \left(\frac{1}{\rho} \frac{d(\rho v)}{dy}\right) + \frac{\rho}{2} \left(\frac{1}{\rho} \frac{d(\rho v)}{dy}\right)^2$$

$$+ 2 \left(\frac{d^2 P}{dx^2}\right) = 0 \qquad (2.32)$$

Y-Momentum

$$\frac{dP}{dy} = 0$$

Energy:

$$\rho v c_p \frac{dT}{dy} = \frac{d}{dy} \left(k \frac{dT}{dy}\right) - \frac{dq_R}{dy} \qquad (2.33)$$

Species Continuity:

$$\rho v \frac{d\tilde{C}_A}{dy} - \frac{d}{dy} \rho \mathcal{D}_{12} \frac{d\tilde{C}_A}{dy} = 0 \qquad (2.34)$$

where $\tilde{C}_A$ is the total elemental concentration of ablation products.

In order to avoid the numerical difficulties which occur when initial value (marching) finite difference approximations are used with mass injection,* this group obtained solutions by beginning the integration of the conservation equations at the stagnation point and proceeding in both directions (toward the wall and toward the shock), and iterating until the boundary conditions at both the wall and shock were satisfied.

The binary diffusion coefficient, $\mathfrak{D}_{12}$, used in Equation 2.34 was that of the C-N interaction. This choice was rather intuitive, but was based upon the fact that the ablation products (carbon-phenolic ablator) consists primarily of carbon while air is predominately nitrogen. It was reported that a posteriori analysis revealed that the choice of the binary diffusion was not critical in the prediction of wall heating rates. For this study, thermodynamic and transport properties of air were used for the injected gases.

The most recent study by Wilson (Ref. 2.16) involves an inviscid analysis of the ablation layer

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*This difficulty is discussed by Rigdon in Reference 2.48 and has been encountered by several other investigators (Refs. 2.14, 2.16, 2.39, 2.41, and 2.43). The difficulties originate from trying to maintain numerical precision when taking small differences between numbers of the same size.

coupled with a viscous analysis of the air layer. In Figure 2.2 the regions of viscous and inviscid flow are graphically illustrated and compared to the assumptions employed by the other investigators. The equations governing the inviscid region are equivalent to those employed by Rigdon, Dirling, and Thomas (Ref. 2.15), with the coefficients of diffusion, viscosity, and thermal conductivity set equal to zero. The following equations correspond to the transformed equations used by Wilson in the ablation layer:

Continuity and X-Momentum:

$$\rho f \frac{d}{dy}\left(\frac{1}{\rho}\frac{d(\rho v)}{dy}\right) = \frac{\rho}{2} \quad \frac{1}{\rho}\left(\frac{d(\rho v)}{dy}\right)^2 + 2\frac{d^2P}{dx^2} \tag{2.35}$$

Y-Momentum:

$$\frac{dP}{dy} = 0 \tag{2.36}$$

Energy:

$$\rho v \frac{dH}{dy} = -\frac{dq_R}{dy} \tag{2.37}$$

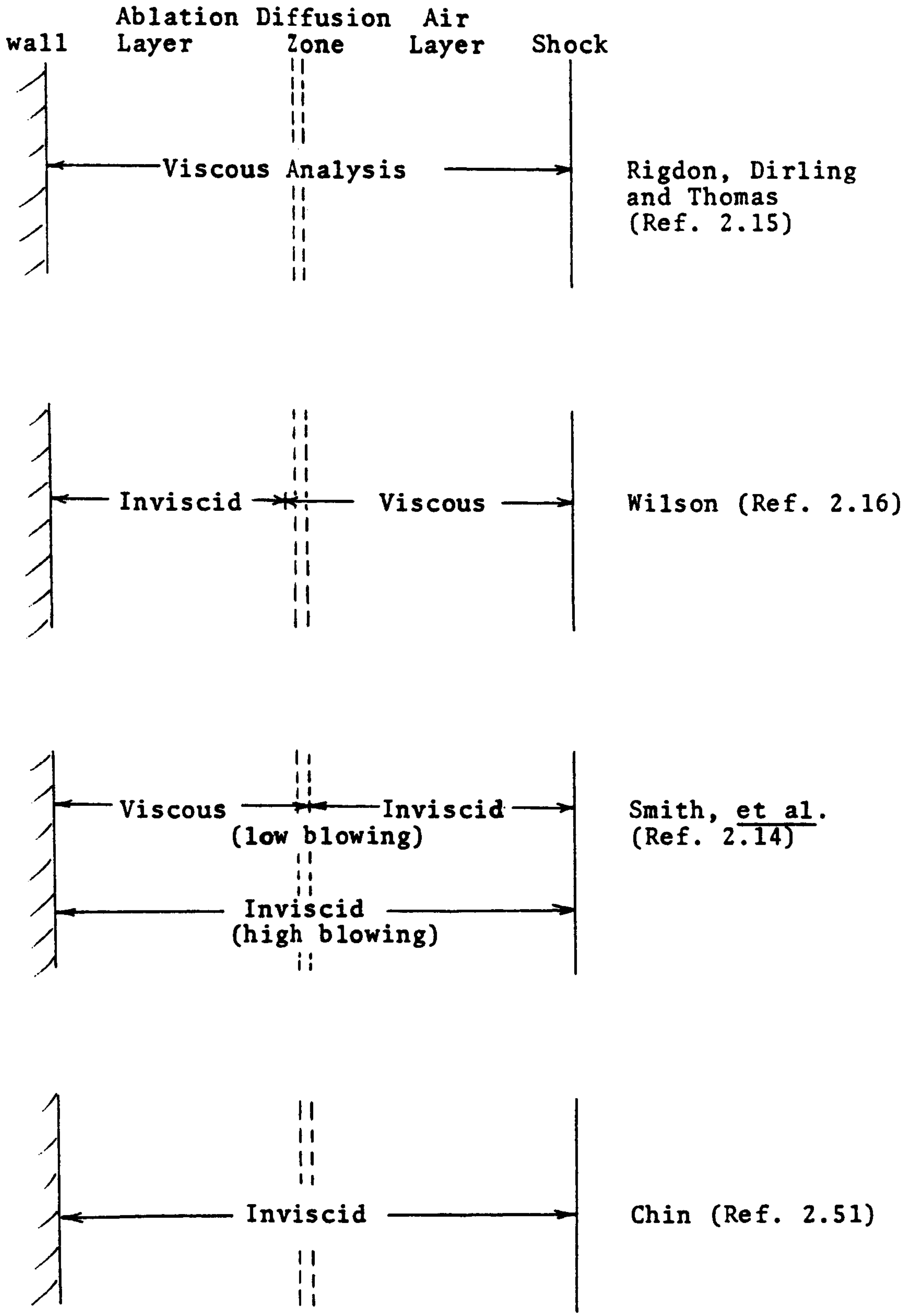

Figure 2.2. Comparison of Radiation Coupled Stagnation Line Analyses with Mass Injection of Ablation Products.

Species Continuity:

$$\frac{d\tilde{C}_A}{dy} = 0 \tag{2.38}$$

In this viscous region, the following equations were transformed and solved:

Continuity and X-Momentum:

$$\frac{d}{dy}\left(\mu \frac{d}{dy}\left(\frac{1}{\rho}\frac{d(\rho v)}{dy}\right)\right) - \rho v \frac{d}{dy}\left(\frac{1}{\rho}\frac{d(\rho v)}{dy}\right) + \frac{\rho}{2}\left(\frac{1}{\rho}\frac{d(\rho v)}{dy}\right)^2 + 2\left(\frac{d^2P}{dx^2}\right) = 0 \tag{2.39}$$

Y-Momentum:

$$\frac{dP}{dy} = 0 \tag{2.40}$$

Energy:

$$\rho v \frac{dH}{dy} = \frac{d}{dy}\left(\frac{\mu}{Pr}\frac{dH}{dy}\right) - \frac{dq_R}{dy} \tag{2.41}$$

Species Continuity:

$$\rho v \frac{d\tilde{C}_A}{dy} - \frac{d}{dy}\left(\rho \mathcal{D}_{12} \frac{d\tilde{C}_A}{dy}\right) = 0 \tag{2.42}$$

In transforming the viscous momentum equation (Eq. 2.39) to the final form required for solution, the assumption was made that the $\rho\mu$ product was constant. Although this assumption resulted in errors as high as 25% (Ref. 2.55) in the velocity profile when compared to a more rigorous solution, no assessment was made of its effects upon a coupled solution. The choice of the binary diffusion coefficient as used in Equation 2.42 was not reported. However, it was stated that the N_2-N interaction was used for the flux term in the prediction of total thermal conductivity (See Appendix A).

Wilson obtained numerical solutions by assuming enthalpy and velocity profiles and performing a forward integration from the wall to the shock, excluding the viscous terms in the ablation layer and including them in the air layer. This procedure was repeated until convergence of the velocity and enthalpy profiles was achieved. The analyses performed included thermodynamic properties of ablation products, but apparently did not include the transport properties of the same species.*

*Wilson's discussion of transport properties is somewhat vague, but includes only references and discussion of air transport data.

The analysis by Smith, et al. (Ref. 2.14) was accomplished by assuming a viscous ablation products region and an inviscid air layer. In this analysis, it was assumed the radiation between the ablation and air layers was uncoupled. For low blowing, the ablation layer was represented by the following equations:*

Continuity:

$$2 \frac{du}{dx} = - \frac{1}{\rho} \frac{d(\rho v)}{dy} \tag{2.43}$$

x-Momentum:

$$\rho v \frac{d}{dy}\left(\frac{du}{dx}\right) - \frac{d}{dy}\left(\mu \frac{d}{dy}\left(\frac{du}{dx}\right)\right) + \rho\left(\frac{du}{dx}\right)^2 + \frac{d^2P}{dx^2} = 0 \tag{2.44}$$

y-Momentum:

$$\frac{dP}{dy} = 0 \tag{2.45}$$

Energy:

$$\rho v \frac{dH}{dy} = \frac{d}{dy}\left(\frac{\mu}{Pr} \frac{dH}{dy}\right) - \frac{dq_R}{dy} \tag{2.46}$$

*These equations are the untransformed equivalents to the final forms employed in the analysis by Smith, et al., (Ref. 2.14). As with the previous discussion of Wilson's study (Ref. 2.16), the equations are presented in this form for comparative purposes.

Elemental Continuity:

$$\rho v \frac{d\tilde{C}_j^2}{dy} - \frac{d}{dy}\,\rho \mathcal{D}_{12} \frac{d\tilde{C}_j}{dy} \qquad j = 1, 2, \ldots, \qquad (2.47)$$

The characteristics of the inviscid air layer were determined by the same set of equations, neglecting the viscous terms as in Equations 2.35 to 2.38.

For large blowing it was assumed that the ablation layer was a region of constant shear and negligible conduction. The elemental compositions were then computed by assuming a cubic relationship in a narrow region between air and ablation layer. With the exception of allowing for an elemental mixing zone, these assumptions result in a completely inviscid analysis for the case of large blowing.* The numerical technique employed in this analysis was a one strip integral technique developed by Suttles in Reference 2.52.

Chin (Ref. 2.51) assumed the entire flowfield to be inviscid with a discontinuous (step function) composition interface between the ablation layer and air

*The mass injection cases reported in Reference 2.14 were apparently solved in this manner.

layer. The equations employed for this study were equivalent to those used by Wilson (Ref. 2.16) and Smith, et al. (Ref. 2.14) for their inviscid regions of analysis. Unlike the analysis of Smith, et al. (Ref. 2.14) the radiative coupling between the ablation and air layers was included. By obtaining solutions in each layer separately while lagging on the solution for the other layer, a fully coupled radiation analysis was obtained.

In a recent study by Page, et al. (Ref. 2.53) of radiation coupled stagnation flow (without mass injection), a comparison was made between their results and those of several other investigators. The comparison included both inviscid and viscous analyses. As shown in Figure 2.3, the results of these investigations are in reasonable agreement. The cases reported by Smith, et al. (Ref. 2.14) all included mass injection and therefore cannot be compared in Figure 2.3. However, comparisons to the results of Chin (Ref. 2.51) and Rigdon, Dirling, and Thomas (Ref. 2.48) were reported in Reference 2.14. For these cases, considerable disagreement in wall heating rates were found (33% and 20% respectively). This discrepancy is most likely due to the fact that the radiation analysis of Smith, et al. does not include line radiation from C and H, both of which are included

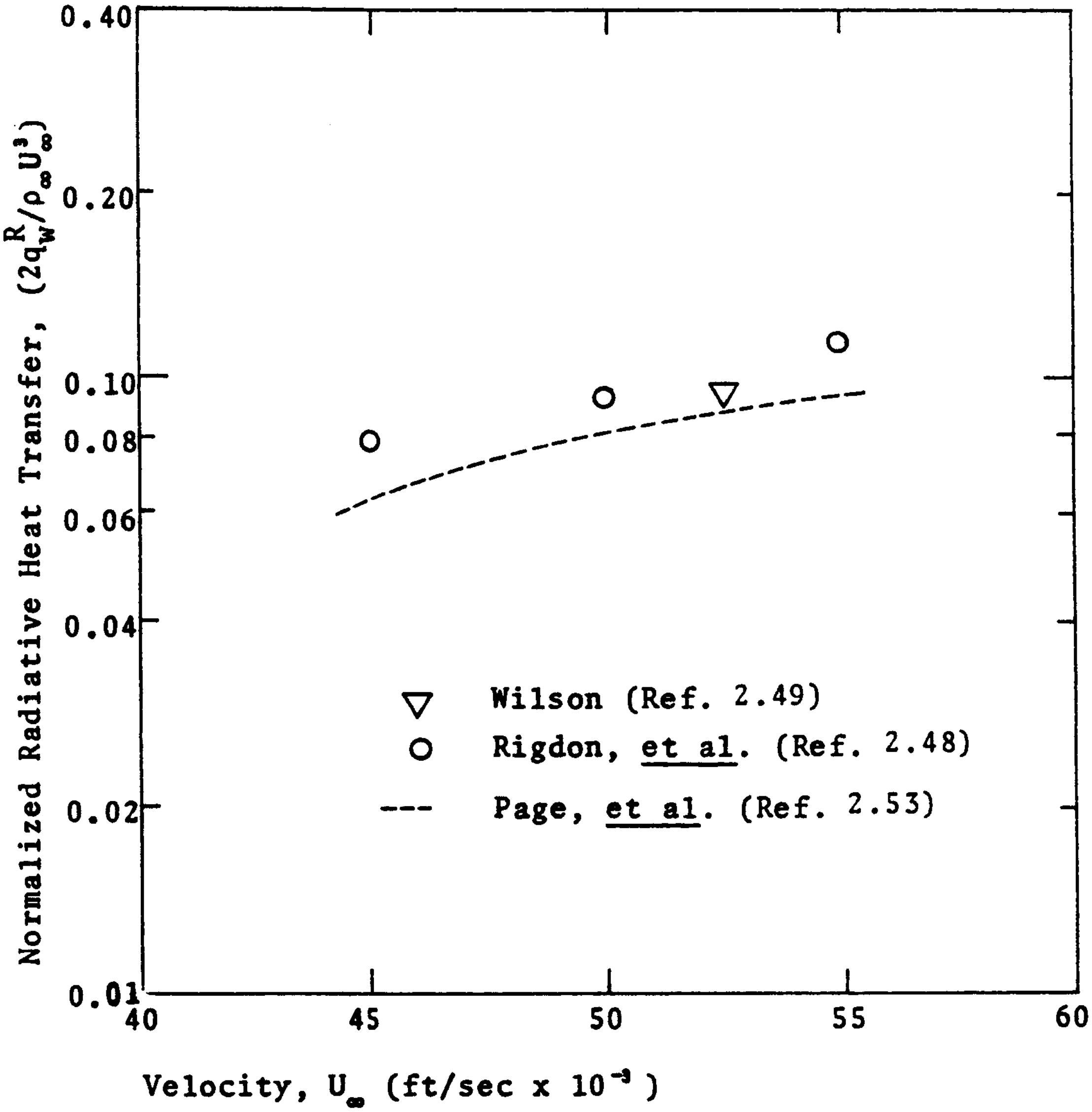

Figure 2.3. Comparison of Dimensionless Radiative Heating Rates (P_S = 1.0 atm., R ≈ 9 ft.)

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in the analyses of Rigdon, et al. (Ref. 2.48), Wilson (Ref. 2.16), Chin (Ref. 2.51), as well as the current study.

Numerical Multicomponent Diffusion Analyses Related to the Study of Ablating Thermal Protection Systems

Relatively few of the studies pertaining to stagnation region heating shields have included multicomponent diffusion effects. A summary of these investigations is given in Table 2.1. Until recently no comparisons between the binary and the multicomponent analyses have been reported. In the past year, the results of two such investigations have been published (Refs. 2.29, 2.43 and 2.44).

In the analysis of Davy, Craig and Lyle (Ref. 2.43), coupled solutions of the transport equations were obtained using both the binary assumption and the Stefan-Maxwell equations to represent the diffusive mass fluxes. Their results confirmed the previously discussed hypothesis that systems of similar molecules would be well represented by the binary approximation. However, for a system containing H_2, N_2, H, and NH_3, the binary approximation gave species profiles which were substantially in error. A general conclusion of this investigation was that a multicomponent solution is required for analyses

TABLE 2.1

A SUMMARY OF RELATED STUDIES WHICH INCLUDE MULTICOMPONENT DIFFUSION

Investigator(s)	System	Diffusion Analysis	Numerical Method
Libby and Pierucci, 1964 (Ref. 2.39)	O_2, H_2, H_2O and N_2	Multicomponent Diffusion Coefficients (Eq. 2.4)	Initial Value With Kutta-Runga-Gil Integration Method
Blotner, 1970 (Ref. 2.54)	N, O, N_2, O_2, NO and NO^+	Multicomponent Diffusion Coefficients	Implicit Two Point Boundary Value Formulation
Nachtsheim, 1967 (Ref. 2.41)	O_2, H_2, H_2O, OH, H, O	Stefan-Maxwell Equations (Eq. 2.5)	Initial Value With Runga-Kutta Startup and Adams-Moulton Continuation
Davy, Craig, and Lyle, 1969 (Ref. 2.43)	(1) NH_3, H_2, H, and N_2 (2) Ar, H_2, H, and N_2 (3) H_2O, H_2, H, OH, N_2, NO, O_2, and O	Stefan-Maxwell Equations	

TABLE 2.1 (continued)

Investigator(s)	System	Diffusion Analysis	Numerical Method
Graves, 1970* (Ref. 2.29)	O_2, H_2, H_2O, and N_2	Stefan-Maxwell Equations	Implicit Two Point Boundary Value Formulation
Present Investigation	O_2, N_2, O, N, O^+, N^+, e^-, H, H_2, CO, C_2, C_3, CN, C_2H, C_2H_2, C_3H, C_4H, HCN, C^+	Exact Effective Diffusion Coefficients Obtained From Stefan-Maxwell Equations	Implicit Two Point Boundary Value Formulation

*Couette flow, ρv = constant.

in which accurate species profiles and local temperatures are important.

The studies by Graves (Ref. 2.29 and 2.44) are perhaps the most valuable with respect to the current investigation. In his analysis of Couette flow with four components, Graves compared three diffusion models: the binary assumption, the bifurication approximation, and the Stefan-Maxwell equations. In conjunction with the binary assumption, a comparison of three methods of estimating a representative diffusion coefficient was also given. The most accurate method for estimating the characteristic binary diffusion coefficient is given as follows:*

$$\mathcal{D}_{12} = 26.28 \times 10^{-4} \frac{T^{3/2}}{P} \sum_{i=1}^{\nu} \frac{Y_i}{\sqrt{M_i}\,\sigma_i^2 \Omega_{ii}^{(1,1)}} \text{ cm}^2/\text{sec} \qquad (2.32)$$

However, the binary model using a diffusion coefficient predicted by this equation gave at best, only a "fair" approximation to the rigorous solution. As mentioned in the previous discussion of the bifurication approximation, the results of the Graves study indicated that the latter approximation gave essentially the same

*An empirical modification of Equation 2.3.

results as the multicomponent diffusion model. It should be pointed out, however, that for the system studied the diffusion factors, F_i (See Equation 2.33), give excellent agreement with the theoretical values of $\mathcal{D}_{ij}$, the maximum error being 2.44%. As shown by Kendall in Reference 2.25, such agreement is certainly not typical since errors as high as 46% were reported.

With the exception of Graves' analysis (Ref. 2.29), all of the previous related studies involving multicomponent diffusion are limited to low mass injection rates, of approximately 1.5% of the free stream mass flux. As previously mentioned, this limitation is characteristic of initial value formulations of problems involving mass injection. The implicit formulation employed in the current study and in the Couette flow study by Graves is not subject to this limitation. Further discussion of these implicit formulations will be included in Chapter V.

Coupled Analyses of the Effects of Transport and Thermodynamic Properties

A survey of the literature revealed only two investigations into the effects of uncertainties in transport and thermodynamic properties upon convective and radiative heating of ablating heat shields. In a study by Howe and Sheaffer (Ref. 2.45), the effect of uncertainties in the thermal conductivity of air on convective heating was examined. Comparing the thermal conductivity models employed by Hansen (Ref. 2.46) and Yos (Ref. 2.47), Howe and Sheaffer found the differences in convective heating to be negligible. However, the resulting temperature profiles were in disagreement by as much as 20%. Such a difference in temperature could greatly effect radiant heating predictions.

Rigdon, Dirling, and Thomas (Ref. 2.15) performed coupled analyses with mass injection of ablation products (carbon phenolic ablator) to determine the effect of using air properties for the ablation products. A comparison of the ratio of these properties in shown in Figure 2.4. The results of their analysis showing the behavior of the radiative flux toward the wall as a function of assumed thermodynamic and transport properties is shown in Figure 2.5. These results indicate that the change in density and heat capacity substantially modified the radiative energy transport in the ablation layer. This phenomena was attributed to the increased absorption (because of the increase in heat capacity) by the injected gases. The negligible effect of the addition of the more

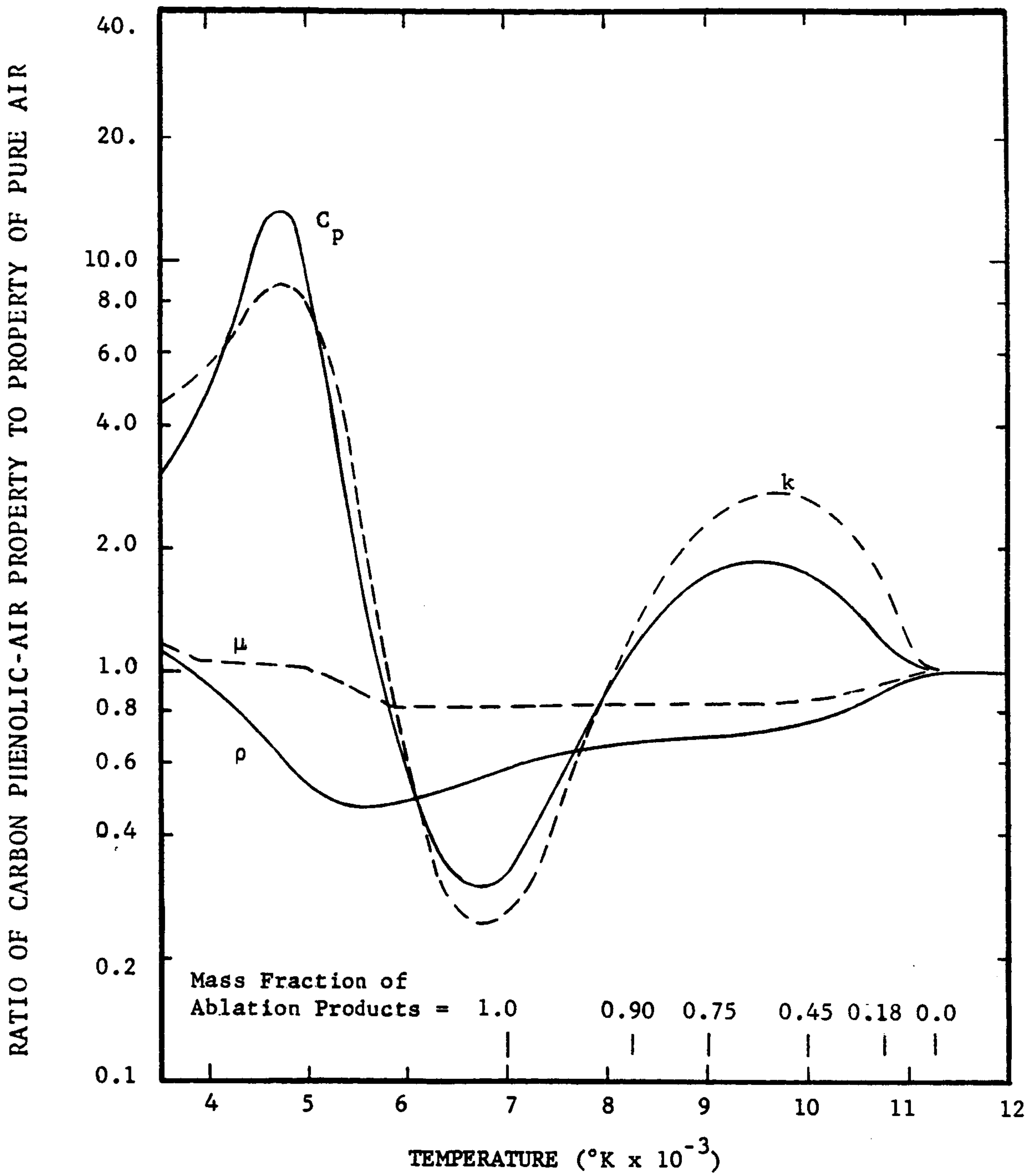

Figure 2.4. Comparison of Properties of Air and Carbon Phenolic-Air Mixture (Ref. 2.15).

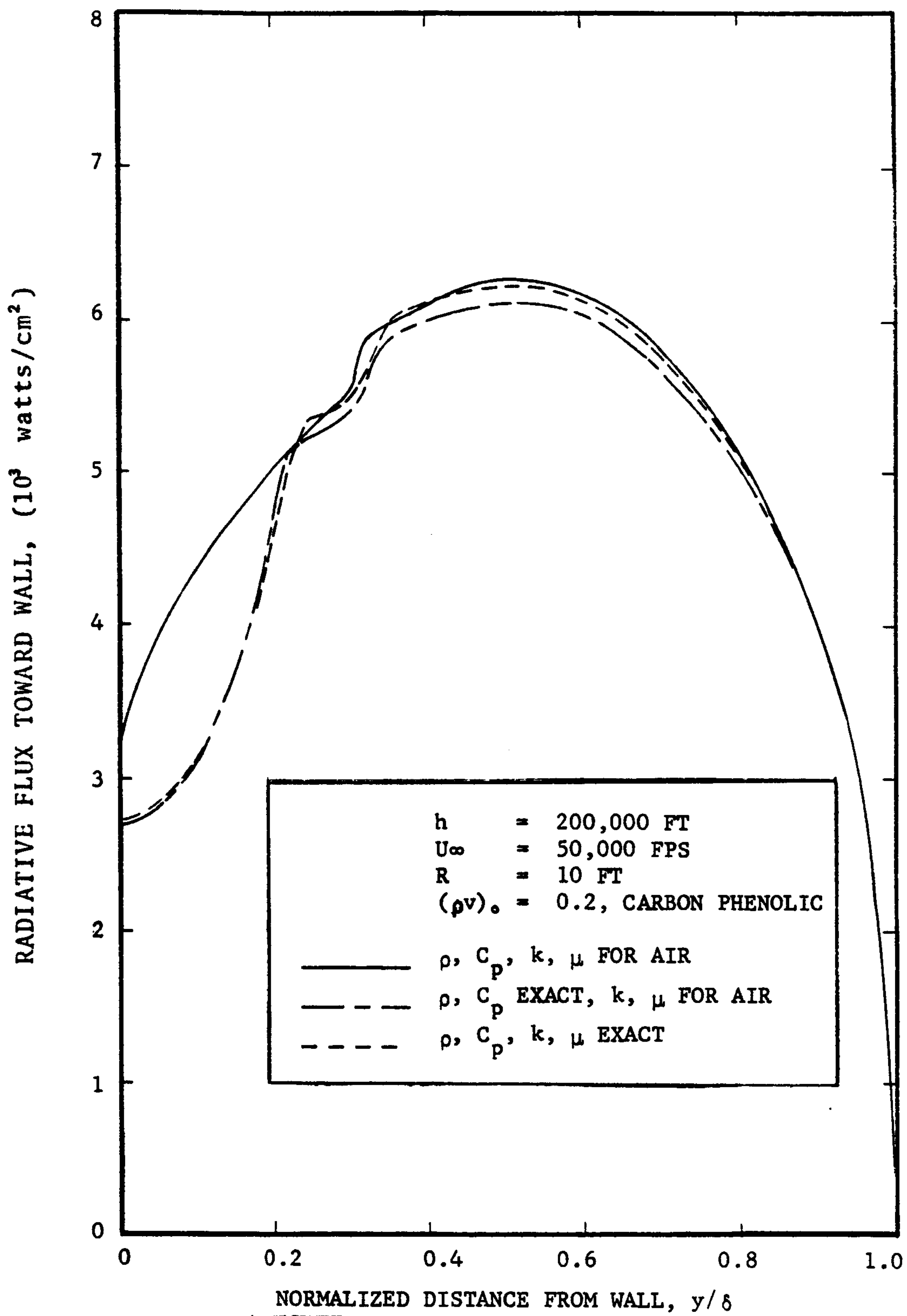

FIGURE 2.5. Effect of Thermodynamic and Transport Properties on the Radiative Flux Toward the Wall.

accurate thermal conductivity was accounted for by the fact that the contribution of this variable is confined to a relatively narrow region around the stagnation point.*

Summary

In this chapter an attempt has been made to perform a detailed survey of the previous work associated with diffusion analyses of multicomponent systems. A survey has been performed of previous investigations into the effects of variations in transport and thermodynamic properties. The primary objective of this review has been that of making an assessment of the relative importance of an exact multicomponent analysis as opposed to approximate methods. Particular emphasis has been given to assessing the reliability of the binary diffusion approximation which has been employed (almost without question) by several major investigators of the blunt-body problem (Refs. 2.13-2.17). From this review it is clear that substantial errors can be introduced in calculations of radiation flowfields through the use of simplified diffusion models. Upon examining the

*This region was referred to as the diffusion zone in Figures 1.2 and 1.3.

currently existing radiation coupled analyses of ablating thermal protection systems, it was found that at best some investigators assume binary diffusion while others neglect diffusion effects entirely.

It was further noted in the review of current radiation heat shield analyses that as a matter of convenience some investigators have assumed the transport properties of air for the ablation layer. Others dispose of the problem entirely by assuming inviscid flow which eliminates all terms containing the transport coefficients. The results of a single study by Rigdon, et al. (Ref. 2.15) suggest that while the proper thermodynamic properties may be important, the differences in transport properties may be of little consequence.

In summary, existing analyses of radiation heating of charring ablators contain several assumptions relating to the transport and thermodynamic properties which have not been thoroughly investigated. As a result, vital questions remain unanswered in the accurate design of ablative thermal protection systems. The major question to be answered by the current study is, "How important are accurate transport and thermodynamic properties in the prediction of radiative heating of charring ablators?" In conjunction with this question, how accurate is a binary diffusion approximation? When are transport (viscous) effects important?

The objectives of this research are to answer these questions by performing theoretical analyses with and without the effects under question, and to thus obtain quantitative estimates of their importance. In so doing, this work will improve the reliability of the results obtained by currently existing analyses and will yield a more thorough understanding of the problems which must be solved in order to obtain more accuracy in the design of ablative thermal protection systems.

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CHAPTER III

DEVELOPMENT OF EQUATIONS FOR A STAGNATION REGION FLOWFIELD ANALYSIS

Introduction

It is the purpose of this chapter to present and develop the necessary equations describing the multicomponent, reacting and radiating flowfield encountered in the aerodynamic heating of ablating, blunt bodies. A detailed development of the governing flowfield equations is presented in Reference 3.1. The development in this reference is a complete derivation of the thin shock layer equations from general transport equations and includes intermediate formulations of varying degrees of rigor. At each stage of the development, the inherent assumptions are indicated so that a logical selection of the appropriate equations can be made.

The following criteria have been established for use in selecting the proper equations for the purposes of this study.

1. Since the most severe heating occurs at and near the leading edge, or stagnation region, of the vehicle special attention should be given to the representation of the flowfield in this vicinity.

2. The equations selected should yield an accurate representation of the flowfield behavior for the body radius and flight conditions selected.

3. The equations must be coupled properly to the surface boundary conditions and must be valid for both large and small mass injection rates.

4. Enough rigor must be maintained such that the effects of diffusion can be properly assessed.

On the basis of these criteria the first order stagnation line, shock layer equations given in Reference 3.1 were selected and will be presented in the following development.

Following the presentation of the stagnation line shock layer equations, several modifications required for each equation will be separately performed and discussed. Subsequently, an analysis of the required boundary conditions for the flowfield equations will be given. Particular emphasis will be directed to the formulation of the surface boundary conditions through which the ablator and flowfield are coupled. The development of the necessary equations will then be concluded by a Dorodnitzyn transformation of the final system of equations to reduce density effects and to place them in final form for a computer solution.

Stagnation Line Thin Shock Equations

A frequently employed simplification in the formulation of hypersonic flow problems is the thin shock layer assumption (Refs. 3.2, 3.7-3.9, 3.13). This assumption implies that the thickness (δ) of the shock layer (the region between the body and shock wave) is much less than the radius of curvature (R) of the adjacent surface. In specific terms, this condition is expressed as,

$$\frac{\delta}{R} << 1 \tag{3.1}$$

For hypersonic flow, it has been shown that the ratio given in Equation 3.1 is of the same order of magnitude as the density ratio across the shock wave, $\bar{\rho}$, (Ref. 3.13). Further, it has been shown that for Re $\geq$ 100,* $\bar{\rho}$ will be of order 0.1 or less. For the flight conditions of interest in the current investigation Reynold's numbers of approximately 10^4 are expected; therefore, the thin shock layer assumption is applicable for the present study.

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*The Reynolds number employed here is based upon the freestream density and velocity, the body radius, and the viscosity on the body side of the shock wave. For typical entry conditions of $U_\infty \approx 50{,}000$ fps, $\rho_\infty = 10^{-5}$ lb/ft^3 and R = 1.0 ft., a value of $T_s \approx 15{,}000$ is obtained therefore $\mu_s \approx 10^{-4}$ lb$_m$/ft^m-sec, and Re$_s \approx 5 \times 10^3$.

Assuming a thin shock layer, an order analysis of the general conservation equations, neglecting all terms less than the order of $\bar{\rho}$, yields the following equations (Refs. 3.1, 3.2, and 3.13):

Global Continuity:

$$\frac{\partial}{\partial x}(\rho r^A u) + \frac{\partial}{\partial y}(\rho \tilde{\kappa} r^A v) = 0 \tag{3.2}$$

Species Continuity:

$$\frac{\partial}{\partial x}(r^A \rho C_i u) + \frac{\partial}{\partial y}(\tilde{\kappa} r^A \rho C_i v) = -\frac{\partial}{\partial y}(\tilde{\kappa} r^A J_{i,y}) + \tilde{\kappa} r^A \omega_i \tag{3.3}$$

x-Momentum:

$$\rho r^A u \frac{\partial u}{\partial x} + \rho \tilde{\kappa} r^A v \frac{\partial u}{\partial y} = -r^A \frac{\partial P}{\partial x} + \frac{\partial}{\partial y}\left[\tilde{\kappa} r^A \mu \frac{\partial u}{\partial y}\right] \tag{3.4}$$

y-Momentum:

$$\rho \kappa u^2 = \tilde{\kappa} \frac{\partial P}{\partial y} \tag{3.5}$$

Energy:

$$r^A \rho u \frac{\partial H}{\partial x} + \tilde{\kappa} r^A \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y}\left(\tilde{\kappa} r^A k_f \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial y}\left(\tilde{\kappa} r^A \sum h_i J_{i,y}\right)$$

$$-\tilde{\kappa} r^A \frac{\partial q_{R,y}^{*}}{\partial y} + \frac{\partial}{\partial y}\left(\tilde{\kappa} r^A \mu u \frac{\partial u}{\partial y}\right) \qquad (3.6)$$

where: $\tilde{\kappa} = 1 + \kappa y$

The body oriented coordinate system and shock layer geometrical relations pertinent to these equations is given in Figure 3.1.

Along the stagnation line, these equations can be simplified to obtain the following:

Global Continuity:

$$2\,\frac{\partial(\rho u)}{\partial x} + \frac{\partial}{\partial y}(\tilde{\kappa}\rho v) + \kappa \rho v = 0 \qquad (3.7)$$

Species Continuity:

$$\tilde{\kappa}\rho v\,\frac{\partial C_i}{\partial y} = -\,\frac{\partial}{\partial y}(\tilde{\kappa} J_i) - \kappa J_i + \tilde{\kappa}\omega_i \qquad (3.8)$$

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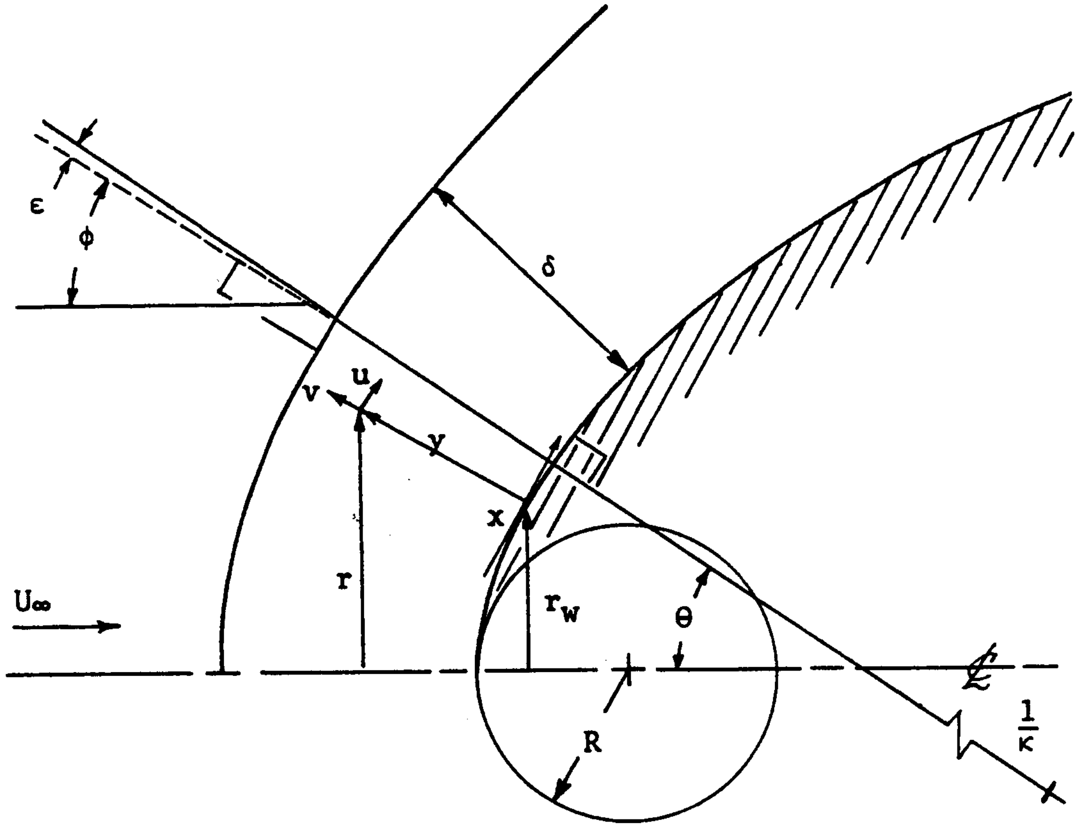
*The term $\partial q_{R,y}/\partial y$ is the radiative flux divergence. The details of its computation are given in Chapter IV.



$$\tan\varepsilon = \frac{d\delta}{(1 + \kappa\delta)\,dx} \qquad \frac{d\theta}{dx} = \kappa(x)$$

$$\delta = \int_0^x (1 + \kappa\delta)\tan\varepsilon\,dx + \delta_0$$

$$\theta = \int_0^x \kappa(x)\,dx$$

Figure 3.1. Body Oriented Coordinate System and Shock Layer Geometrical Relations.

x-Momentum:

$$\frac{\partial}{\partial y}\left[\tilde{\kappa}\mu\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)\right] + [\kappa\mu - \tilde{\kappa}\rho v]\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$$

$$- \kappa\left[\rho v + \mu\frac{\kappa}{\tilde{\kappa}} + \frac{1}{2}\frac{\partial \mu}{\partial y}\right]\left(\frac{\partial u}{\partial x}\right) - \rho\left(\frac{\partial u}{\partial x}\right)^2$$

$$- \frac{\partial^2 P}{\partial x^2} = 0 \qquad (3.9)$$

y-Momentum:

$$\frac{\partial P}{\partial y} = 0 \qquad (3.10)$$

Energy:

$$\tilde{\kappa}\rho v\frac{\partial H}{\partial y} = -\left(1 + \frac{\kappa}{\tilde{\kappa}}\right)\frac{\partial}{\partial y}\left[-\tilde{\kappa}k\frac{\partial T}{\partial y} + \tilde{\kappa}\sum h_i J_i\right]$$

$$- \tilde{\kappa}\frac{\partial q_R}{\partial y} \qquad (3.11)$$

Since the boundary layer thickness is small in comparison to the local body radius (Eq. 1.1), the following additional simplifications exist:

$$\kappa \cong 0 \qquad (3.12)$$

$$\tilde{\kappa} \cong 1 \qquad (3.13)$$

Applying these simplifications to Equations 3.7-3.11, the first order stagnation line, thin shock equations are obtained:

Global Continuity:

$$2\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial}{\partial y}(\rho v) \tag{3.14}$$

Species Continuity:

$$\rho v\frac{\partial C_i}{\partial y} = -\frac{\partial J_i}{\partial y} + \omega_i \qquad i=1, 2, \ldots, \nu \tag{3.15}$$

x-Momentum:

$$\frac{\partial}{\partial y}\left[\mu\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)\right] - \rho v\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right) - \rho\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial^2 P}{\partial x^2}\right)_{x=0} = 0 \tag{3.16}$$

y-Momentum:

$$\frac{\partial P}{\partial y} = 0 \tag{3.17}$$

Energy:

$$\rho v\frac{\partial H}{\partial y} = -\frac{\partial}{\partial y}\left[-k\frac{\partial T}{\partial y} + \sum h_i J_i\right] - \frac{\partial q_R}{\partial y} \tag{3.18}$$

In the sections to follow the fomulation of these equations will be further developed to obtain more convenient forms for numerical solutions.

<u>Species Equations</u>. For studies of reacting flow systems in chemical equilibrium, a useful simplification which eliminates the reaction rate term in the species equation can be realized by transforming the ν species equations (Eqs. 3.15) to elemental equations. The transformation, referred to as the Shvab-Zeldovich transformation (Refs. 3.3-3.5), is accomplished by means of the following relationships:

$$\tilde{C}_j = \tilde{M}_j \sum_{i=1}^{\nu} \frac{A_{ij} C_i}{M_i} = \text{mass fraction of element } j \tag{3.19}$$

$$\tilde{J}_j = \tilde{M}_j \sum_{i=1}^{\nu} \frac{A_{ij} J_i}{M_i} = \text{mass flux of element } j \tag{3.20}$$

where A_{ij} represents the moles of element j per mole of compound i, $\tilde{M}_j$ is the atomic weight of the element j and M_i is the molecular weight of the compound i. The details of the transformation are given in Appendix A. The resulting form of the elemental conservation equations is

$$\rho v \frac{d\tilde{C}_j}{dy} = - \frac{d\tilde{J}_j}{dy} \qquad j = 1, 2, \ldots, \ell \tag{3.21}$$

The species mass flux, J_i, appearing in Equation 3.15 is generally computed by assuming binary (Fick's Law) diffusion (Refs. 3.7-3.10):

$$J_i = - \rho \mathcal{D}_{12} \frac{dC_i}{dy} \tag{3.22}$$

where a single diffusion coefficient, $\mathcal{D}_{12}$, is chosen to represent the diffusive behavior of all species in the system. As shown in Appendix A, the binary flux expression (Eq. 3.22) can be conveniently transformed by the Shvab-Zeldovich transformation to an elemental basis.

$$\tilde{J}_j = - \rho \mathcal{D}_{12} \frac{d\tilde{C}_j}{dy} \tag{3.23}$$

This relationship can be substituted into the elemental continuity equations (Eqs. 3.21) to yield the following second order ordinary differential equations,

$$\rho v \frac{d\tilde{C}_j}{dy} = \rho \mathcal{D}_{12} \frac{d^2\tilde{C}_j}{dy^2} + \frac{d(\rho \mathcal{D}_{12})}{dy} \frac{d\tilde{C}_j}{dy} \qquad j = 1, 2, \ldots, \tag{3.24}$$

or

$$\frac{d^2\tilde{C}_j}{dy^2} + p(y)\,\frac{d\tilde{C}_j}{dy} = 0 \qquad j = 1, 2, \ldots \ell \tag{3.25}$$

where

$$p(y) = \frac{d\ln\mathcal{D}_{12}}{dy} + \frac{d\ln\rho}{dy} - \frac{v}{\mathcal{D}_{12}} \tag{3.26}$$

For situations, such as the current study, where more accuracy is required in determining species distribution, the Stefan-Maxwell equations can be utilized to compute the diffusive mass fluxes. The Stefan-Maxwell Equations were presented in the Chapter II (Eq. 2.5) as follows:

$$\frac{dY_i}{dy} = \sum_{i=1}^{\nu} \frac{Y_i Y_j}{\mathcal{D}_{ij}} (V_j - V_i) \qquad i = 1, 2, \ldots, \nu-1 \tag{2.5}$$

As discussed in the previous chapter, these equations do not form an independent set. It is therefore necessary to replace one of the Stefan-Maxwell Equations by Equation 2.13:

$$\sum_{i=1}^{\nu} \rho_i V_i = \sum_{i=1}^{\nu} J_i = 0 \tag{2.13}$$

Unfortunately, the resulting system of ν equations which accurately describes the multicomponent diffusion velocities cannot be simplified by means of the Shvab-Zeldovich transformation. However, it is still possible, as will be demonstrated in Chapter V, to use the present forms of Equations 2.5 and 2.13 with the elemental equations (Eqs. 3.21) to obtain accurate species distributions in equilibrium flow.

Momentum Equation. To obtain a more classical form of the momentum equation a velocity function ($\mathcal{f}'$) is defined

$$\mathcal{f}' = \frac{\partial u}{\partial x} \Big/ \left(\frac{\partial u}{\partial x}\right)_s \tag{3.27}$$

where the quantity $\left(\frac{\partial u}{\partial x}\right)_s$ is the tangential velocity gradient at the shock and can be determined from the Rankine-Hugoniot Equations (to be subsequently discussed). Substituting Equation 3.27 into the momentum equation (Eq. 3.16) gives the following:

$$\frac{d}{dy}\left(\mu \frac{d\mathcal{f}'}{dy}\right) - \rho v \frac{d\mathcal{f}'}{dy} - \rho \left(\frac{\partial u}{\partial x}\right)_s (\mathcal{f}')^2 - \frac{\partial^2 P}{\partial x^2} = 0 \tag{3.28}$$

The tangential pressure gradient term appearing in this equation is a function of the flow downstream and consequently cannot be rigorously determined without an analysis of the downstream effects. It has been shown that for a thin shock layer, this term is constant along the stagnation line (Ref. 3.1) and therefore can be evaluated at any point. From the Rankine-Hugoniot Equations the pressure behind the shock can be expressed as

$$P_s = [(1 - \bar{\rho}) \cos^2 \phi]\rho_\infty U_\infty{}^2 \qquad (3.29)$$

differentiaion yields

$$\frac{\partial^2 P_s}{\partial x^2} = - 2(1 - \bar{\rho}) \left(\frac{\partial \phi}{\partial x}\right)^2 [\cos^2 \phi - \sin^2 \phi] \rho_\infty U_\infty{}^2 \qquad (3.30)$$

An approximation of a concentric shock is consistent with the thin shock layer analysis. For a concentric shock, $\left(\frac{d\phi}{dx}\right)_{x=0} = 1$ (See Figure 3.1). Furthermore, $\phi = 0$ at $x = 0$. Therefore, Equation 3.30 becomes

$$\left(\frac{\partial^2 P}{\partial x^2}\right)_{x = 0} = - 2 (1 - \bar{\rho}) \rho_\infty U_\infty{}^2 \qquad (3.31)$$

Substituting Equation 3.31 into the momentum equation (Eq. 3.27), the following equation is obtained:

$$\frac{d}{dy}\,\mu\,\frac{d\mathcal{f}'}{dy} - \rho v\frac{d\mathcal{f}'}{dy} - \rho\left(\frac{\partial u}{\partial x}\right)_s (\mathcal{f}')^2 + 2\,(1 - \bar{\rho})\,\rho_\infty U_\infty^2 = 0 \tag{3.32}$$

A simultaneous solution of the above equation with the Global Continuity Equation (Eq. 3.14), expressed in terms of $\mathcal{f}'$ (Eq. 3.27), thus defines the velocity distribution. The necessary form of the Global Continuity Equation is given as follows:

$$2\,\mathcal{f}'\left(\frac{\partial u}{\partial x}\right)_s = -\frac{1}{\rho}\frac{d}{dy}\,(\rho v) \tag{3.33}$$

<u>Energy Equation</u>: Since the available thermodynamic and transport properties* are expressed in terms of temperature, it is desirable to reformulate the energy equation in terms of temperature rather than enthalpy as the dependent variable. The required manipulations for this conversion are given in Reference 3.6 and are shown in the development to follow.

Consider the term on the left hand side of Equation 3.18,

$$\rho v\frac{dH}{dy} = \rho v\frac{d}{dy}\left(h + \frac{u^2 + v^2}{2}\right) \tag{3.34}$$

*Presented in Chapter IV.

Noting that

$$h = \sum_{i=1}^{\nu} C_i h_i \tag{3.35}$$

$$\frac{dh}{dy} = \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} + \left(\sum_{i=1}^{\nu} C_i \frac{dh_i}{dT} \right) \frac{dT}{dy} \tag{3.36}$$

$$\frac{dh}{dy} = \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} + \left(\sum C_i c_{p_i} \right) \frac{dT}{dy}$$

$$\frac{dh}{dy} = \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} + c_{pf} \frac{dT}{dy} \tag{3.37}$$

Substitution of Equation 3.37 into Equation 3.33 and noting that $u = 0$ at $x = 0$ gives,

$$\rho v \frac{dH}{dy} = \rho v \left[\sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} + c_{pf} \frac{dT}{dy} + \frac{d}{dy} \left(\frac{v^2}{2} \right) \right] \tag{3.38}$$

Combining Equations 3.38 and 3.18 yields

$$\rho v c_{pf} \frac{dT}{dy} = \frac{d}{dy} \left(k_f \frac{dT}{dy} \right) - \rho v \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} - \rho v^2 \frac{dv}{dy}$$

$$- \frac{d}{dy} \left(\sum_{i=1}^{\nu} h_i J_i \right) - \frac{dq_R}{dy} \tag{3.39}$$

In the experimental measurement of the thermal conductivity and heat capacity of gaseous mixtures, certain effects attributed to the reactive behavior of the mixture are observed. As will be illustrated by the following development, these effects are predicted by the energy equation, but are not included in the terms normally associated with ordinary thermal conductivity and heat capacity. Therefore it is convenient to incorporate the additional terms into these coefficients for consistency with experimental observations.

The quantities c_{p_f} and k_f appearing in Equation 3.39 are referred to respectively as the "frozen" heat capacity and thermal conductivity. As shown in Appendix B, the summation terms of Equation 3.39 can be rearranged to combine with the above coefficients to yield the following form of the energy equation:

$$\rho v\ c_p \frac{dT}{dy} = \frac{d}{dy}\left(k\frac{dT}{dy}\right) - \rho v^2 \frac{dv}{dy} - \frac{dq_R}{dy} \tag{3.40}$$

where

$$c_p = c_{p_f} + \sum h_i \left(\frac{\partial C_i}{\partial T}\right) \tag{3.41}$$

and

$$k = k_f + \rho \sum D_i h_i \left(\frac{\partial C_i}{\partial T}\right) \tag{3.42}$$

As given in the preceding equation, the total heat capacity, c_p, includes the effects of chemical heats of reaction as an additional mechanism of energy absorption. The total thermal conductivity, k, accounts for the additional transport of energy through the diffusion of high energy molecules into regions of lower energy. This effect is not to be confused with the related phenomena of thermal diffusion which accounts for the flux of mass due to temperature gradients.

For a fully coupled analysis, it is important that the behavior of the ablative material be properly incorporated in the formulation. In the current investigation, the contribution of the ablator appears as a boundary condition to the flowfield equations. A derivation of these relationships is given in the following discussion.

Derivation of Surface Interaction Relations

The boundary conditions for this investigation can be derived in either of two ways. The first, and most frequently used, technique consists of simply formulating a physical balance across the boundaries of the system. A second technique involves the use of the flowfield equations themselves, which are integrated across the system boundaries and then contracted by taking the limit as the spacial increment approaches zero. Both of these methods should yield identical results. In this development both of these techniques will be employed. The first method has the advantage that the physical significance of each term in the resulting equation is more readily evident. The second, the integration technique, will assure that all of the necessary terms have been considered.

<u>Species Boundary Conditions</u>: At the char surface the following general surface balance is applicable:

$$\left[\begin{array}{l}\text{convective flux}\\ \text{of species i on}\\ \text{the char side}\\ \text{of the interface}\end{array}\right] + \left[\begin{array}{l}\text{diffusive flux}\\ \text{of species i on}\\ \text{the char side}\\ \text{of the interface}\end{array}\right] + \left[\begin{array}{l}\text{all contribu-}\\ \text{tions to the}\\ \text{net flux of}\\ \text{species i due}\\ \text{to surface}\\ \text{phenomena}\end{array}\right]$$

$$= \left[\begin{array}{l}\text{convective flux}\\ \text{of species i on}\\ \text{flowfield side}\\ \text{of the interface}\end{array}\right] + \left[\begin{array}{l}\text{diffusive}\\ \text{flux of}\\ \text{species i}\\ \text{on flow-}\\ \text{field side}\\ \text{of the}\\ \text{interface}\end{array}\right] . \qquad (3.43)$$

or

$$\rho v C^- + J_i^- + S_i = \rho v C_i^+ + J_i^+ \qquad (3.44)$$

The surface generation (S_i) can now be quantitatively defined and the remaining terms of the equation verified by examining an integral derivation of this relationship. It can be shown that the following equation describes the heterogeneous system which exists at the char interface:

$$\rho v \frac{dC_i}{dy} = - \frac{dJ_i}{dy} + \omega_{i_{homo}} + \omega_{i_{hetero}} + \omega_{i_{subl}} \qquad (3.45)$$

In this relationship, both the solid and gas phases have been included. As shown in Figure 3.2, the following overall material balance exists at the surface:

$$(\rho v)_{wall} = \rho_g v_g + \rho_c v_r = \text{mass injection rate} \qquad (3.46)$$

The generation terms appearing in Equation 3.45 are defined as follows

$\omega_{i_{homo}}$ = net generation of species i by means of homogeneous chemical reactions (3.47)

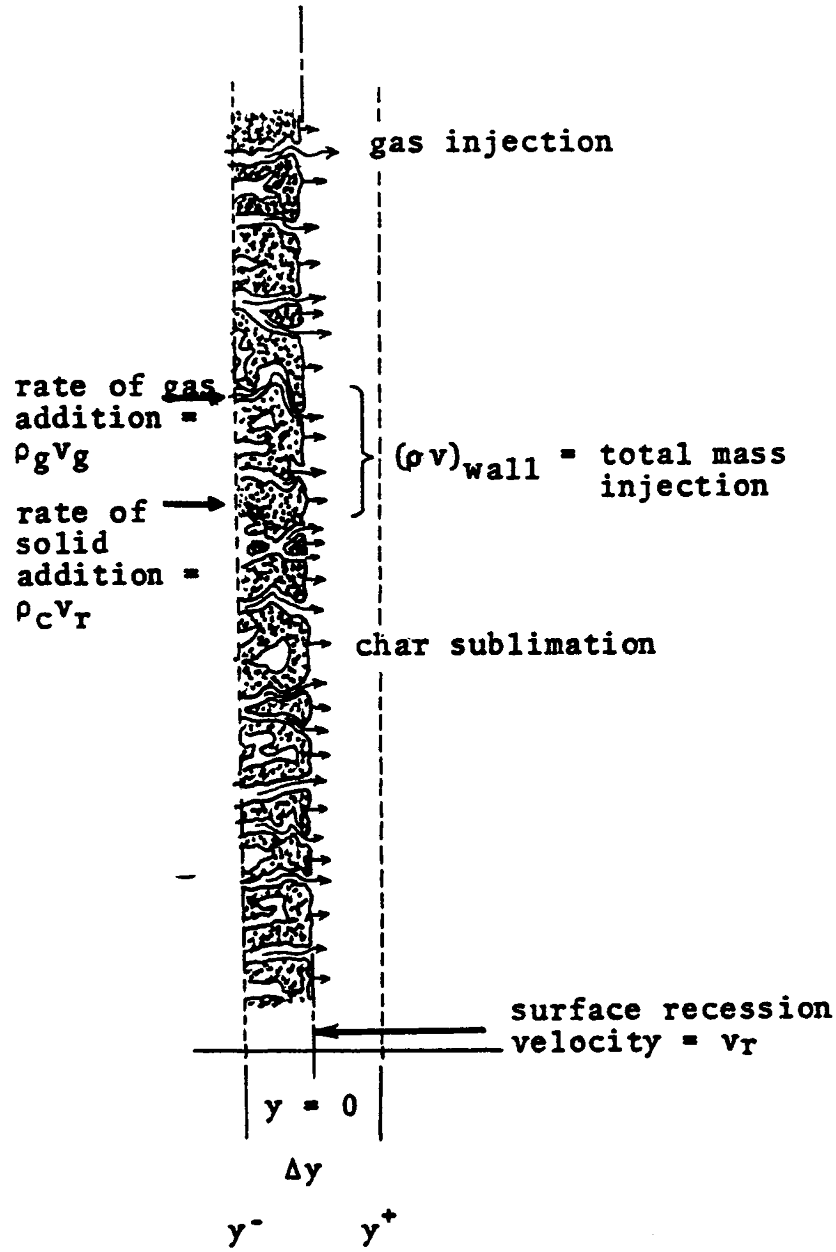


Figure 3.2. Illustration of Overall Surface Material Balance.

$\omega_{i_{hetero}}$ = net generation of species i by means of heterogeneous reactions (excluding sublimation) (3.48)

$\omega_{i_{subl}}$ = net generation of species i by means of sublimation of the solid phase (3.49)

Each of the previous terms represents a generation of mass of species i by reaction per unit time per unit volume. For the ablator this unit volume contains both gas and solid. Thus if r_i is the rate of formation of species i by heterogeneous reaction per unit area of solid surface, A_T, then $\omega_{i_{hetero}}$ is given by the following equation:

$$\omega_{i_{hetero}} = \frac{r_i A_T}{A \Delta y} \tag{3.50}$$

The ratio of $A_T/A\Delta y$ represents the concentration of surface area, i.e., the area of available surface per unit volume of the reacting system. In the subsequent steps of this analysis Equation 3.45 will be integrated across the char interface a distance of Δy which will define the thickness of a control volume of cross-sectional area A which contains a total reactive surface area A_T. Equation 3.50 can also be conveniently expressed in terms of char porosity, (volume of voids per unit volume), which for an isotropic material is equal to $(A - A_T)/A$. Thus,

$$\omega_{i_{hetero}} = r_i\ (1 - \varepsilon_p)/\Delta y \qquad (3.51)$$

In a similar manner the sublimation term can be derived as,

$$\omega_{i_{subl}} = s_i\ (1 - \varepsilon_p)/\Delta y \qquad (3.52)$$

where s_i, is the mass rate of sublimation per unit area of solid surface. The homogeneous reaction rate term represents the net rate of formation of species i in the gas phase and requires no rearrangement.

Having now defined, quantitatively, the total generation term in the species continuity equation, the integration technique will be used to define s_i in terms of w_i. Equation 3.45 can be integrated as follows:

$$\int_{y^-}^{y^+} \rho v \frac{dC_i}{dy}\ dy = -\int_{y^-}^{y^+} \frac{dJ_i}{dy}\ dy + \int_{y^-}^{y^+} \left(\omega_{i_{homo}} + \omega_{i_{hetero}} + \omega_{i_{subl}}\right) dy \qquad (3.53)$$

Substituting Equations 3.51 and 3.52, into the above gives:

$$\int_{y^-}^{y^+} \rho v dC_i = - \int_{y^-}^{y^+} dJ_i + \int_{y^-}^{y^+} \omega_{i_{homo}} \, dy$$

$$\int_{y^-}^{y^+} (r_i + s_i)\,(1 - \varepsilon_p)\, dy \qquad (3.54)$$

Integrating the above equation noting that ρv is a constant gives

$$\rho v C_i^+ - \rho v C_i^- = J_i^- - J_i^+ + (\omega_{i_{homo}})_{mean}\, \Delta y + (r_i + s_i)(1 - \varepsilon_p) \qquad (3.55)$$

Taking the limit as $\Delta y \to 0$, and rearranging gives:

$$\rho v C_i^- + J_i^- + (r_i + s_i)\,(1 - \varepsilon_p) = \rho v C_i^+ + J_i^+ \qquad (3.56)$$

Comparing the above equation with Equation 3.44 confirms our previous surface balance and defines, S_i the dimensionless surface generation term as:

$$S_i = (r_i + si)\ (1 - \varepsilon_p)$$

Although Equation 3.57 is completely rigorous for all species which may exist either in the flow-field or the char, a more specific interpretation of this equation can be arrived at for various types of species which can be grouped into distinct categories. For example: pyrolysis gases (excluding carbon), carbon gas, all remaining gases, and finally the solid carbon.

Elemental Boundary Conditions. Following the procedure of Appendix A, the species boundary condition equations can be transformed to elemental boundary conditions. Multiplication of Equation 3.56 by the appropriate elemental distributions and summing over the species gives

$$\rho v \sum_{i=1}^{\nu} e_{ij} C_i^- + \sum_{i=1}^{\nu} e_{ij} J_i^- = \rho v \sum_{i=1}^{\nu} e_{ij} C_i^+ + \sum_{i=1}^{\nu} e_{ij} J_i^+ \qquad (3.58)$$

which can be expressed in terms of elemental mass fractions, $\tilde{C}_j$ and elemental mass fluxes, $\tilde{J}_j$.

$$\rho v \tilde{C}_j^- + \tilde{J}_j^- = \rho v \tilde{C}_j^+ + \tilde{J}_j^+ \tag{3.59}$$

The above equations are the elemental surface boundary conditions and represent a significant simplification over the species surface boundary conditions since the generation terms have been eliminated.*

<u>Energy Boundary Conditions</u>. Starting with Equation 3.18 the energy balance at the surface will be developed in a fashion analogous to the preceding one for the species equations.

$$\rho v \frac{dH}{dy} = - \frac{d}{dy}\left[- k_f \frac{dT}{dy} + \sum_{i=1}^{\nu} h_i J_i \right] - \frac{dq_R}{dy} \tag{3.18}$$

Integrating the above equation across the char surface gives

$$\rho v \ (H^+ - H^-) = \left[k_f \frac{dT}{dy} - \sum_{i=1}^{\nu} h_i J_i \right]^+ - \left[k \frac{dT}{dy} - \sum_{i=1}^{\nu} h_i J_i \right]^- - q_R^+ + q_R^- \tag{3.60}$$

*It should be noted that Equations 3.56 and 3.59 are both boundary conditions of the third kind since $\tilde{J} = \tilde{J}\ (d\tilde{C}/dy)$. The specific treatment of this difficulty is given in Chapter V.

The above equations can be placed in a more convenient form using the following equations. The equation for the total enthalpy is

$$H = h + \frac{v^2}{2g_c} \tag{3.61}$$

and, using the definition of the static enthalpy it can be written in terms of the mass fraction, C_i, and enthalpy per unit mass of i, h_i.

$$H = \sum_{i=1}^{\nu} h_i C_i + \frac{v^2}{2g_c} \tag{3.62}$$

Noting that kinetic energy terms are small compared to the enthalpy terms and can be deleted, the left hand side of Equation 3.60 can be written as

$$\rho v \ (H^+ - H^-) = \rho v \sum h_i (C_i^+ - C_i^-) \tag{3.63}$$

The terms on the right hand side of Equation 3.60 will now be evaluated. As discussed previously and is shown in Appendix B, the bracketed terms can be expressed in terms of the total thermal conductivity.

$$\left[k_f \frac{dT}{dy} - \sum h_i J_i \right] = k \frac{dT}{dy} \tag{3.64}$$

Substitution of Equations 3.63 and 3.64 into Equation 3.60 gives the following form of the energy surface balance:

$$\rho v \sum h_i \; (C_i^+ - C_i^-) = k^+ \frac{dT}{dy}\Big|^+ - k_b^- \frac{dT}{dy}\Big|^- - q_R^+ \qquad (3.65)$$

where k_b^- is the bulk thermal conductivity of the char for which experimental values are available (Ref. 3.12). These values thus account for all modes of heat transfer in the porous media, including the radiant effect, q_R^-.

Momentum Boundary Conditions. Integration of the stagnation line y-momentum equation (Eq. 3.17) yields the following simple result:

$$p^- = p^+ \qquad (3.66)$$

In summary, the derivation of the stagnation line surface boundary conditions have been presented. It should be noted that, since u = 0 at the interface for all x, these same boundary conditions are applicable around the body. This extension can be confirmed by performing the previous analysis with the more general two-dimensional boundary layer equations.

Ablator Response and the Quasi-steady Assumption

In the previous section boundary conditions were derived to describe the interaction between a gaseous flowfield and a moving solid-gas interface. To predict the overall heat shield requirements for a particular entry trajectory, a transient (unsteady-state) analysis can be performed. Such an analysis would involve the solution of a set of partial differential equations describing the unstead ablator response to a heat pulse determined by the trajectory. An alternate approach to this unsteady analysis is a quasi-steady analysis which is described in the following discussion.

A schematic diagram of the zones occuring in a charring ablator is given in Figure 3.3. Also shown are typical temperature and density profiles in the material. The virgin plastic decomposes in a distinct zone in a temperature range from about 700°K to 1300°K, and in this region the density decreases from that of the virgin plastic of about 35 lb/ft^3 to that of the char of about 14 lb/ft^3 for a nylon-phenolic resin composite.

During the heating of the material the surface is removed by chemical reactions (e.g., oxidation),

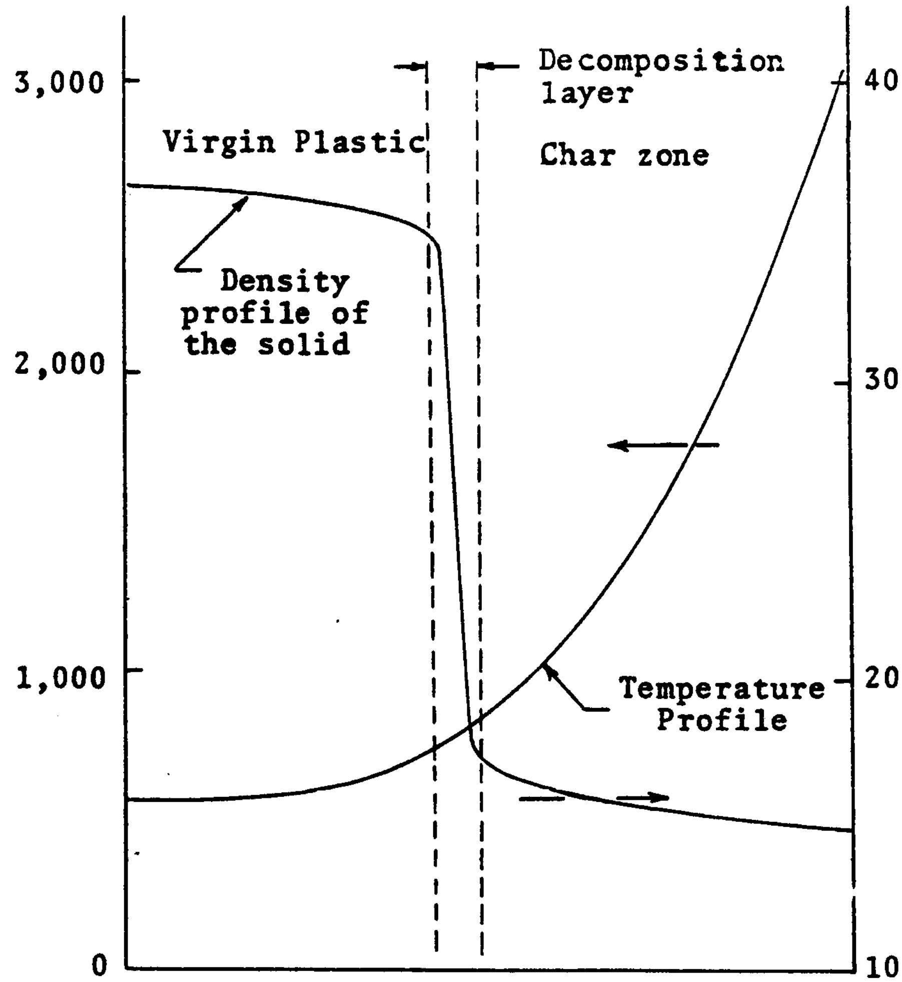


Figure 3.3. Illustration of Typical Density and Temperature Profiles in an Ablative Composite.

sublimation and erosion. As a result the total thickness of material decreases as is shown by the data in Figure 3.2. At the same time the decomposition in depth is occurring, and a char layer builds up. It is not unusual to have the rate of surface removal being equal to the rate of decomposition after an initial, transient initial period. Under these conditions a constant char layer thickness, z, and a constant surface recession velocity, v_r, are maintained after this initial period.

The previously described phenomena is referred to as a "quasi-steady state" (Refs. 3.15 and 3.16) and permits a steady state analysis of the ablator response. Assuming a quasi-steady state, an overall material balance on the ablator can be written as follows (see Figure 3.5):

$$\rho_o v_r = \rho_c v_r + \rho_g v_g \tag{3.67}$$

$$\rho_o v_r = (\rho v)_w = \text{mass injection rate wall} \tag{3.68}$$

i.e., the mass flux of virgin plastic ($\rho_o v_r$) is equal to the blowing rate, $(\rho v)_w$.

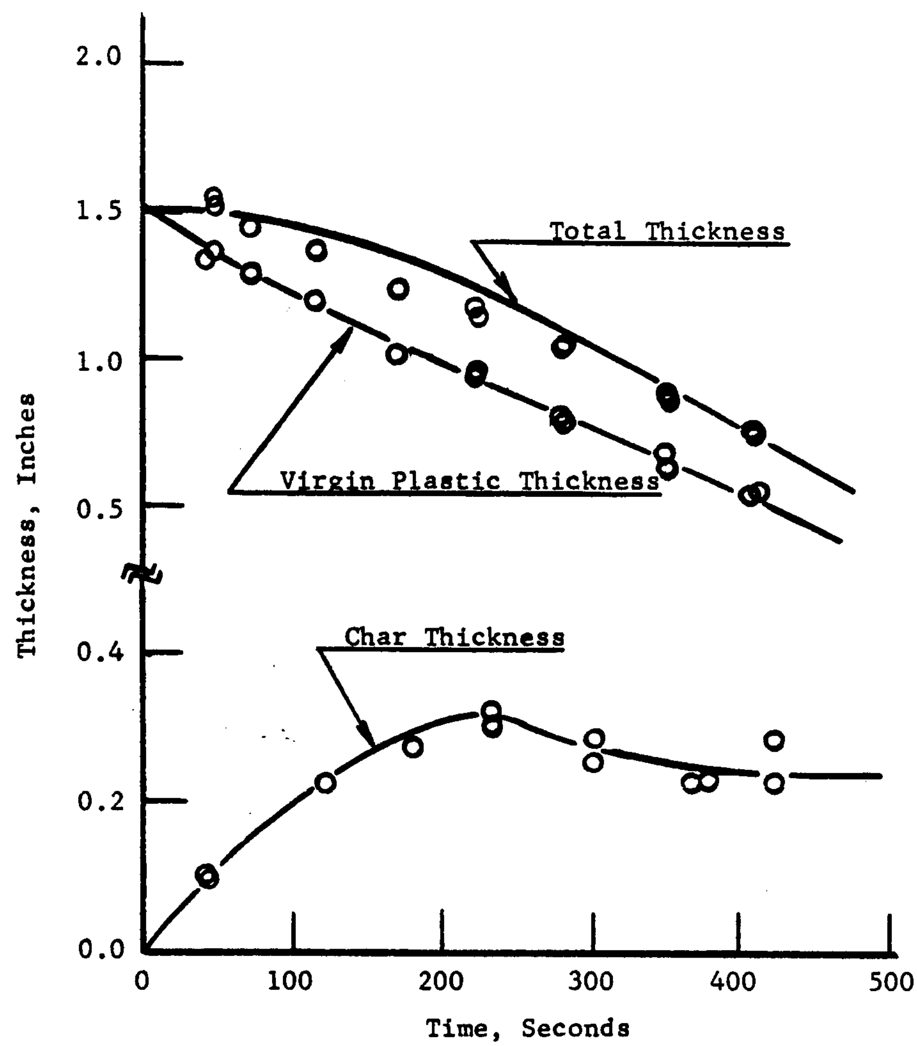


Figure 3.4. Thickness of the Char and Virgin Plastic as a Function of Time (Ref. 3.14).

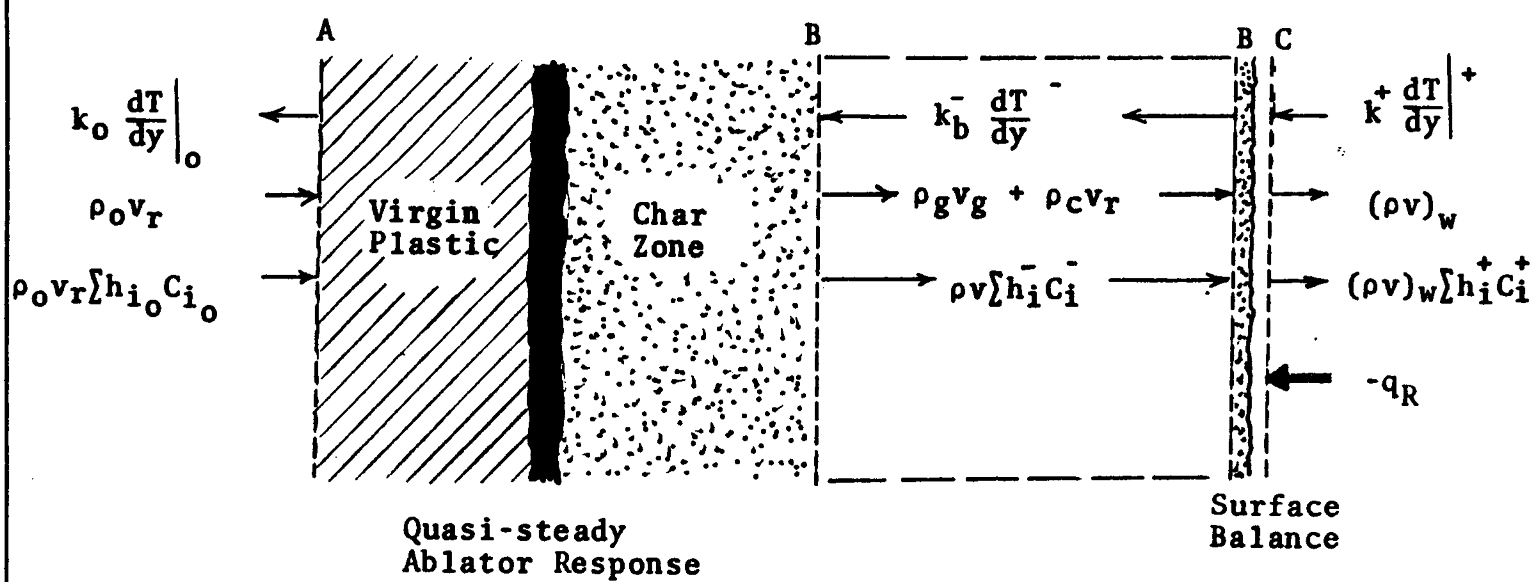


Figure 3.5. Illustration of Flowfield Coupling and Quasi-steady Ablator Response.

The overall energy balance on the ablator becomes (See Fig. 3.5):

$$k_b^- \left.\frac{dT}{dy}\right|^- + \rho_o v_r \sum_{i=1}^{\nu} h_{i_o} C_{i_o} = k_o \left.\frac{dT}{dy}\right|_o + \rho v \sum_{i=1}^{\nu} h_i^- C_i^- \tag{3.69}$$

when Equation 3.69 is combined with the energy surface balance (Eq. 3.65), a useful relationship between the surface heating and the ablator response is obtained:

$$q_T = \Delta H_{ablation} \, (\rho v)_w + k_o \left.\frac{dT}{dy}\right|_o \tag{3.70}$$

where

$$q_T = q_R^+ + k^+ \left.\frac{dT}{dy}\right| = \text{total heat input to ablator surface} \tag{3.71}$$

and

$$\Delta H_{ablation} = \sum_{i=1}^{\nu} h_i^+ C_i^+ - \sum_{i=1}^{\nu} h_{i_o} C_{i_o} \tag{3.72}$$

[heat of ablation]

For chemical equilibrium, the heat of ablation can be determined from a specified temperature in the virgin plastic and the surface temperature of the ablator which is equal to the sublimation temperature of char. For a given ablator, the sublimation temperature is a function of the flowfield pressure which in turn is determined by the altitude and velocity of the entering vehicle. Therefore, given a pressure at the ablator surface, a fixed relationship (Eq. 3.70) exists between the mass injection rate and total surface heating. This relationship is given for a phenolic-nylon ablator in Figure 3.6 for several surface pressures and the corresponding temperatures. In general, the heat conducted into the virgin plastic is less than 1% of the total heat absorbed by the ablator. Although not specifically included in the results of Figure 3.6 its addition would not change the results shown here.

Shock Boundary Conditions

From the shock geometry and the Rankine-Hugoniot equations (Ref. 3.13) the shock boundary conditions can be determined. In Reference 3.1, these equations are given in rectangular coordinates as shown below.

Continuity:

$$\rho_\infty V_\infty = \rho_S V_S \tag{3.73}$$

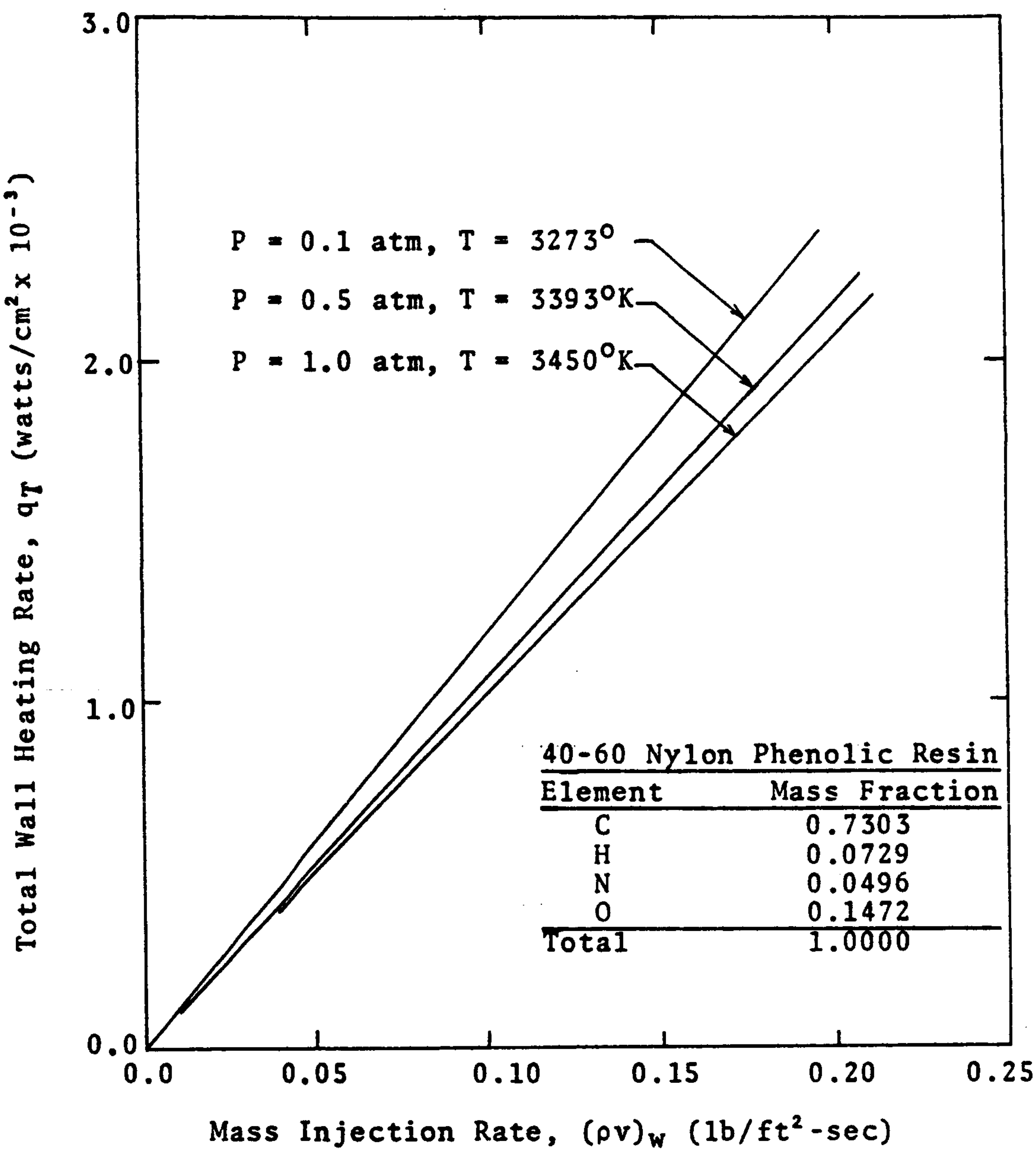


Figure 3.6. Equilibrium Mass Injection Rates Versus Wall Heating Rates for Various Surface Pressures and Corresponding Temperatures.

Momentum:

$$\text{(normal)}\ \rho_\infty V_\infty^2 + P_\infty = \rho_s V_s^2 + P_s \tag{3.74}$$

$$\text{(tangential)}\ V_\infty = V_s \tag{3.75}$$

Energy:

$$\frac{1}{2} V_\infty^2 + h_\infty = \frac{1}{2} V_s^2 + h_s \tag{3.76}$$

Upon transforming to curvilinear coordinates and non-dimensionalizing using dimensionless groups given in Table 3.1, the Rankine-Hugoniot equations can be written as (Ref. 3.11):

$$v_s = \sin \phi \sin \varepsilon - \bar{\rho} \cos \phi \cos \varepsilon \tag{3.77}$$

$$u_s = \sin \phi \cos \varepsilon + \bar{\rho} \cos \phi \sin \varepsilon \tag{3.78}$$

$$P_s = (1 - \bar{\rho}) \cos^2 \phi \tag{3.79}$$

$$h_s = (1 - \bar{\rho}^2) \cos^2 \phi = 1 - (u_s^2 + v_s^2) \tag{3.80}$$

For a stagnation line solution, the shock boundary conditions are determined by evaluating the above equations at $y = \delta$ and $x = 0$, with the following results:

$$v = v_s = -\bar{\rho} \tag{3.81}$$

$$u = u_s = 0 \tag{3.82}$$

$$P = P_s = 1 - \bar{\rho} \tag{3.83}$$

$$h = h_s = 1 - \bar{\rho} = 1 - v_s^{2} \tag{3.84}$$

Assuming that pure air in chemical equilibrium exists at the shock, the edge boundary conditions for the species equations are thus available from an equilibrium calculation.

$$C_i = C_{i,s} = f\,(P_s,\ h_s) \tag{3.85}$$

Nondimensionalization and Transformation of the Flowfield Equations

As a matter of convenience, the final forms of the previously given flowfield equations (Eqs. 2.5, 3.14, 3.17, 3.21, and 3.40), can be nondimensionalized, using the dimensionless groups defined in Table 3.1 to yield the following set of equations:*

Continuity:

$$2f' \left(\frac{\partial u}{\partial x}\right)_s = -\frac{1}{\rho}\ \frac{d}{dy}\ (\rho v) \tag{3.86}$$

---

*For the remainder of this chapter, all dimensional quantities will be labeled with the symbol, (˚) as employed in Table 3.1.

TABLE 3.1.

DIMENSIONLESS GROUPS USED FOR NONDIMISIONALIZATION OF THE GOVERNING TRANSPORT EQUATIONS

$$u = \frac{\dot{u}}{\dot{U}_\infty}^{*} \qquad v = \frac{\dot{v}}{\dot{U}_\infty} \qquad p = \frac{\dot{p}}{\dot{\rho}_{s,o}\dot{U}_\infty^{2}} \qquad \rho = \frac{\dot{\rho}}{\dot{\rho}_{s,o}}$$

$$x = \frac{\dot{x}}{\dot{r}_\omega} \qquad y = \frac{\dot{y}}{\dot{r}_\omega} \qquad \mu = \frac{\dot{\mu}}{\dot{\mu}_{s,o}} \qquad T = \frac{\dot{T}}{\dot{T}_{s,o}}$$

$$h = \frac{\dot{h}\ \dot{g}c}{\frac{1}{2}\dot{U}_\infty^{2}} \qquad c_p = \frac{\dot{c}_p\ \dot{T}_{s,o}\dot{g}c}{\frac{1}{2}\dot{U}_\infty^{2}} \qquad k = \frac{\dot{k}\ \dot{T}_{s,o}\dot{g}c}{\dot{R}\ \dot{\rho}_{s,o}\ \dot{U}_\infty^{3}}$$

$$J_i = \frac{\dot{J}_i}{\dot{\rho}_{s,o}\ \dot{U}_\infty} \qquad \omega_i = \frac{\dot{r}_w\ \dot{\omega}_i}{\dot{\rho}_{s,o}\dot{U}_\infty} \qquad \frac{dq_R}{dy} = \frac{\frac{d\dot{q}_R}{d\dot{y}}\ \dot{r}_\omega}{\dot{\rho}_{s,o}\ \dot{U}_\infty^{3}}$$

$$Re_s = \frac{\dot{\rho}_{s,o}\ \dot{U}_\infty\ \dot{r}_w}{\dot{\mu}_{s,o}} \qquad D = \frac{\dot{D}}{\dot{r}_\omega\ \dot{U}_\infty}^{**} \qquad V_i = \frac{\dot{V}_i}{\dot{U}_\infty}$$

* (˙) designates dimensional quantities.

**This nondimensionalization of diffusion coefficient is used for all forms (multicomponent, binary, and effective).

Species Continuity:

$$\rho v \frac{dC_i}{dy} = - \frac{dJ_i}{dy} + \omega_i \qquad i = 1, 2, \ldots, \nu \quad (3.87)$$

Elemental Continuity:

$$\rho v \frac{d\tilde{C}_j}{dy} = - \frac{d\tilde{J}_j}{dy} \qquad i = 1, 2, \ldots, \quad (3.88)$$

Stefan-Maxwell:

$$\frac{dY_i}{dy} = \sum_{i=1}^{\nu} \frac{Y_i Y_j}{\mathcal{D}_{ij}} (V_j - V_i) \quad i = 1, 2, \ldots, \nu - 1 \quad (3.89)$$

x-Momentum:

$$\frac{1}{\mathbf{Re}_s} \frac{d}{dy} \left(\mu \frac{df'}{dy} \right) - \rho v \frac{df'}{dy} - \rho \left(\frac{\partial u}{\partial x} \right)_s (f')^2 \frac{2\bar{\rho}(1 - \bar{\rho})}{(\partial u/\partial x)_s} = 0 \quad (3.90)$$

Y-Momentum:

$$\frac{dP}{dy} = 0 \quad (3.91)$$

Energy:

$$\frac{\rho v c_p}{2} \frac{dT}{dy} = \frac{d}{dy} \left(k \frac{dT}{dy} \right) - \rho v^2 \frac{dv}{dy} - \frac{dq_R}{dy} \quad (3.92)$$

These equations can now be transformed using the Dorodnitzyn transformation. This transformation is employed to reduce the effects of the large variations in density and is written as follows:

$$\eta = \frac{\int_0^y \rho dy}{\int_0^\delta \rho dy} = \frac{\int_0^y \rho dy}{\tilde{\delta}} \qquad (3.93)$$

which yields upon differentiation,

$$\frac{d}{dy} = \frac{\rho}{\tilde{\delta}} \frac{d}{d\eta} \qquad (3.94)$$

Transforming Equations 3.86 through 3.92 by means of Equation 3.94 gives*

Global Continuity:

$$2\ f' \left(\frac{\partial u}{\partial x}\right)_s = -\frac{1}{\tilde{\delta}} \frac{d}{d\eta} (\rho v) \qquad (3.95)$$

Species Continuity:

$$\rho v \frac{dC_i}{d\eta} = -\frac{dJ_i}{d\eta} + \frac{\omega_i \tilde{\delta}}{\rho} \qquad i = 1, 2, \ldots, \nu \qquad (3.96)$$

---

*In the transformed equations, the quantity f' is defined as $\rho \mathcal{f}'/\tilde{\delta}$.

Elemental Continuity:

$$\rho v \frac{d\tilde{C}_j}{d\eta} = - \frac{d\tilde{J}_j}{d\eta} \qquad j = 1, 2, \ldots, \ell \tag{3.97}$$

Stefan-Maxwell:

$$\frac{dY_i}{d\eta} = \frac{\tilde{\delta}}{\rho} \sum_{i=1}^{\nu} \frac{Y_i Y_j}{\mathcal{D}_{ij}} (V_j - V_i) \qquad i = 1, 2, \ldots, \nu - 1 \tag{3.98}$$

x-Momentum:

$$\frac{d}{d\eta}\left(\rho\mu\frac{df'}{d\eta}\right) - \rho v \, Re_s \, \tilde{\delta} \, \frac{df'}{d\eta} + \frac{Re_s \; 2\bar{\rho}(1-\bar{\rho}) - \rho\frac{\partial u}{\partial x}\Big|_s^2 (f')^2}{\rho \left(\frac{\partial u}{\partial x}\right)_s} = 0 \tag{3.99}$$

y-Momentum:

$$\frac{dP}{d\eta} = 0 \tag{3.100}$$

Energy:

$$\frac{1}{2}\rho v c_p \frac{dT}{d\eta} \quad \frac{d}{d\eta}\left(\frac{k\rho}{\tilde{\delta}} \; \frac{dT}{d\eta}\right) - \rho v^2 \frac{dv}{d\eta} - \frac{dq_R}{d\eta} \tag{3.101}$$

The above set of coupled, first and second order, ordinary differential equations are the final form of the stagnation line thin-shock equations. From these equations the temperature, pressure, composition, and velocity profiles for a multicomponent reacting, and radiating chemical system can be determined. The specific way that these equations are solved with the boundary conditions is given in the discussion of numerical implementation in Chapter V.

Summary

The necessary flowfield equations and boundary conditions required for a coupled radiation analysis of stagnation region heating of ablating thermal protection systems have been presented. These equations have been further developed to a formulation which is more convenient for numerical implementation. Before discussing the details of numerical solutions, it is important that the transport, thermodynamic, and radiative properties which determine the coefficients and sources terms (in the case of radiation) of the equations be properly assessed. Therefore, the chapter to follow will contain a detailed evaluation of these properties. It will then be appropriate in Chapter V to pursue the numerical solution of these equations on a digital computer.

3

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CHAPTER IV

TRANSPORT, THERMODYNAMIC, AND RADIATIVE PROPERTIES

Theoretical Predictions of High Temperature Gas Properties

The reliability of the flowfield calculations in the current study is highly dependent on the values used for the various transport, thermodynamic, and radiative properties. With this in mind, it is desirable to attain the ultimate in accuracy; however, some complications do exist. There is very little data in the temperature range of interest in this work, and the data that does exist is subject to some scrutiny due to experimental difficulties at these higher temperatures. Therefore, it becomes necessary to rely heavily on rigorous kinetic theory and statistical thermodynamics for the estimation of these properties.

Transport Properties

Generally, investigators in this area have resorted to the classical Chapman-Enskog kinetic theory relations for estimation of the required transport properties. The modification of these relationships to account for polyatomic, reacting mixtures results in very cumbersome equations. In some cases, as will be shown, there are simplifications which can be applied without substantial loss in accuracy. At this point, it becomes desirable to optimize between accuracy and computation time. A wide variety of methods for estimating these properties has been developed in just this manner. In this section, a formulation is provided from which an optimum method to accurately compute high temperature transport properties with reasonable computational convenience is developed.

At the lower temperatures where ionization has not yet begun to occur, the classical first order Chapman-Enskog kinetic theory relations have been found to be reasonably accurate. However, for partially and fully ionized gases, more rigorous expressions are required. An evaluation of these methods is given by Ahtye in Reference 4.1. On the basis of the available data, the estimations obtained from higher order kinetic theory analyses are quite good. Several such comparisons are given by Ahtye in the previously mentioned technical note. In the discussion to follow, the sources of theoretical estimates for the required properties of viscosity, thermal conductivity and binary diffusion coefficients are given and the methods of computer implementation for each of these properties are discussed.

Viscosity: For computer implementation the data obtained from theoretical predictions was curve fitted to a second order polynomial.

$$\mu_i = a_i + b_i T + c_i T^2 \tag{4.1}$$

Data for air species was taken from Yan, *et al*. (Ref. 4.2). The estimated viscosities of the ionized species, N^+, O^+, and e^-, were obtained from the air mixture properties reported by Yos (Ref. 4.6). The procedure for arriving at these estimates will be subsequently discussed. Figure 4.1 shows a comparison of this data and the resulting curve-fits. Viscosity predictions for the ablation products were taken from a number of sources (Refs. 4.3-4.5). The data and corresponding correlations for each of these species are given in Figure 4.2. No data was available for the species, C_2H, C_3H, and C_4H. Therefore, on the basis of molecular weight, C_2H was assumed to have the transport properties of CN; C_3H and C_4H were assumed to have the same properties as C_3.

The relationship employed for the prediction of mixture viscosity was the commonly used Buddenberg-Wilke correlation (Ref. 4.6).

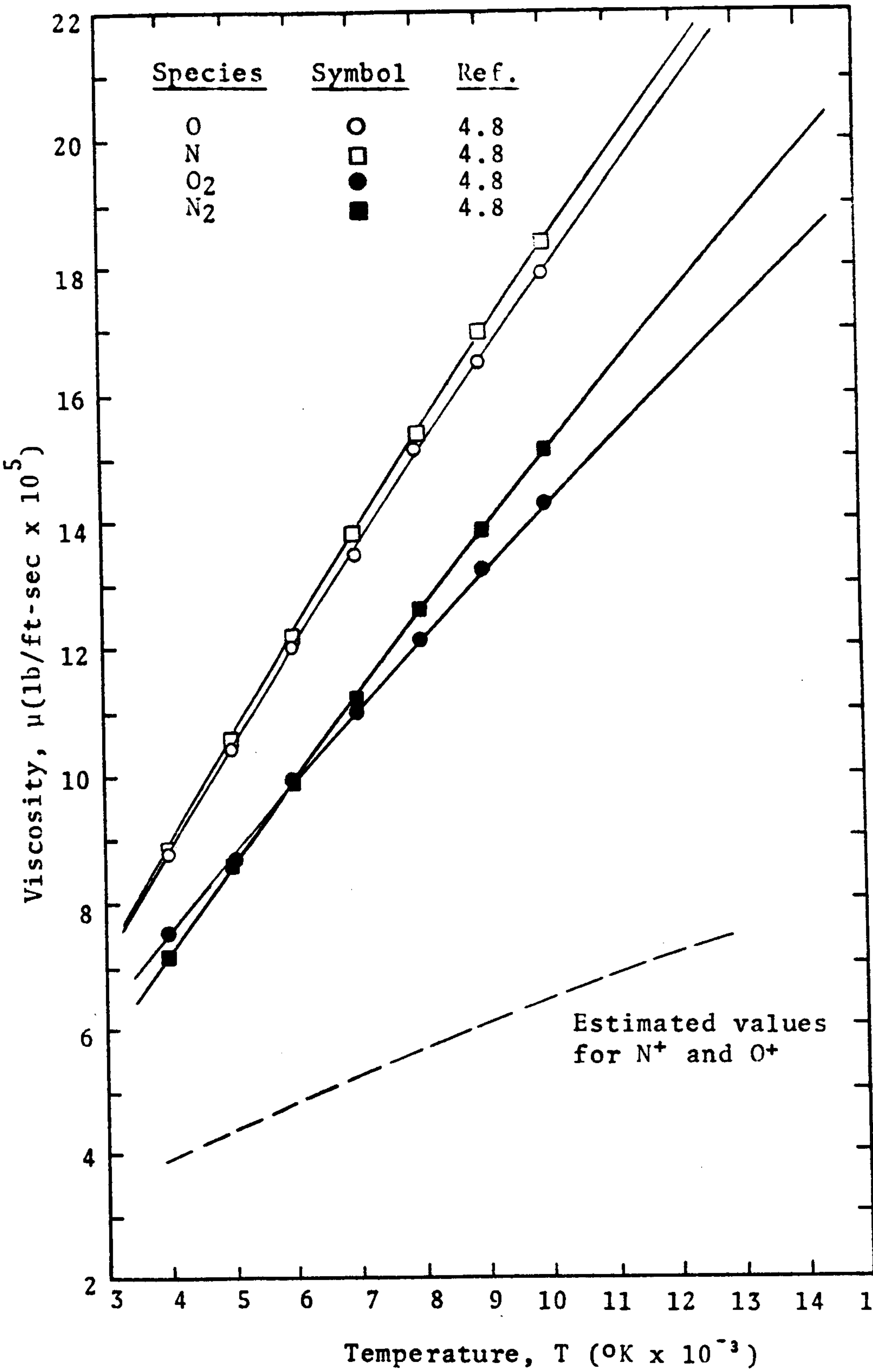


Figure 4.1 Viscosity of Air Species at 1.0 Atm.

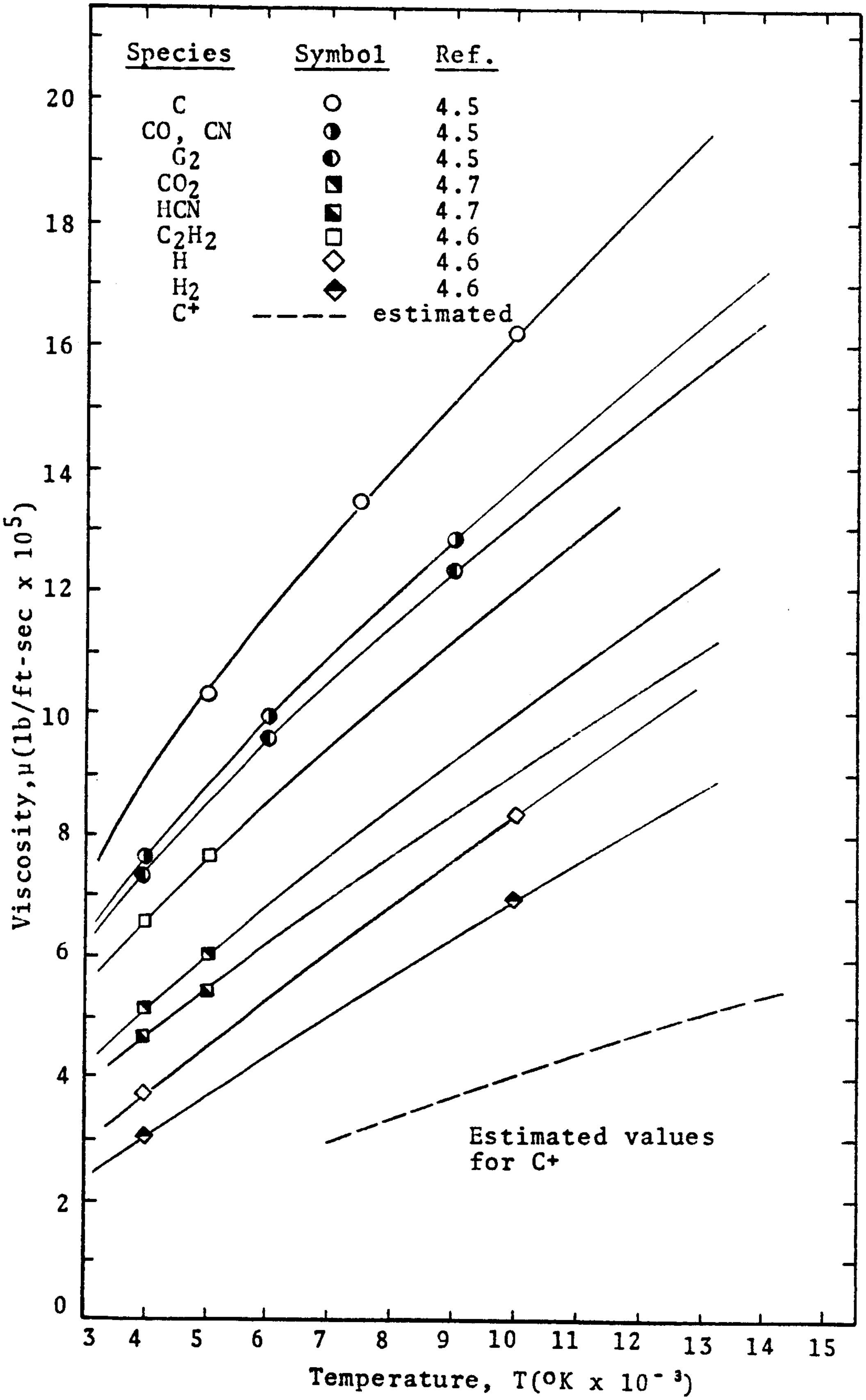


Figure 4.2. Viscosity of Ablation Products at 1 atm.

$$\mu = \sum_{i=1}^{\nu} \frac{Y_i \mu_i}{\sum_{j=1}^{\nu} Y_j \Phi_{ij}} \tag{4.2}$$

where

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j}\right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}\right]^2 \tag{4.3}$$

The results for air viscosity using this correlation are presented in Figure 4.3 and compared with those obtained from more rigorous procedures. The excellent agreement obtained for the sub-ionization temperatures (less than 9000°K at 1.0 atm) demonstrates the capabilities of the Buddenberg-Wilke correlation in predicting gas mixture properties. The viscosity and frozen thermal conductivity predictions of Yos (Ref. 4.7) and of Lee and Bobbitt (Ref. 4.8) were obtained from a more rigorous formulation than those of Hansen (Ref. 4.9). For temperatures exceeding 9000°K agreement with the results of Yos (Ref. 4.7) was accomplished by adjusting the values of the properties of N^+, O^+ and e^-. In this manner, the properties of these species were estimated. It was further assumed that C^+ would exhibit similar behavior and could therefore be represented by the same

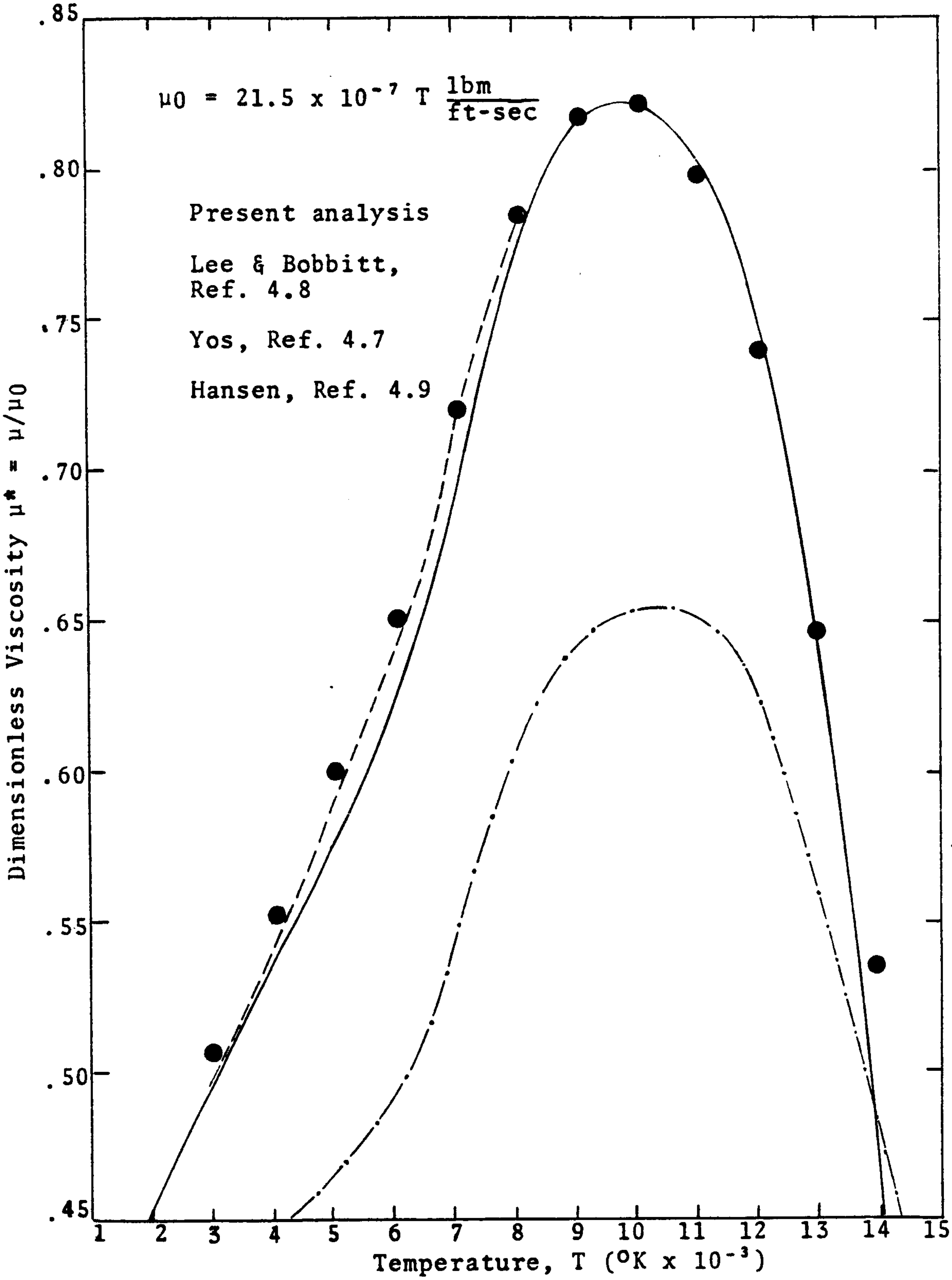


Figure 4.3. Viscosity of Air at One Atmosphere.

properties as the previously discussed ionized components. A summary of the empirical constants required for Equation 4.1 is given in Table 4.1.

Thermal Conductivity: As with the viscosity data, theoretical predictions of frozen thermal conductivities of air species were obtained from Reference 4.2. The resulting data is given in Figure 4.4. Examination of the data revealed that a linear fit would be satisfactory for accurate correlation:

$$k_i = a_i + b_i T \tag{4.4}$$

Corresponding data for the ablation products were collected from References 4.3, 4.4, and 4.5 and are shown in Figure 4.5. As with viscosity, the thermal conductivities of the ionized species were determined from air mixture properties of Yos (Ref. 4.7). A summary of the coefficients required for Equation 4.4 is given in Table 4.2. Mixture thermal conductivity was calculated in the same manner as mixture viscosity:

$$k_f = \sum_{i=1}^{\nu} \frac{Y_i k_i}{\sum_{j=1}^{\nu} Y_i \Phi_{ij}} \tag{4.5}$$

TABLE 4.1

EMPIRICAL CONSTANTS FOR VISCOSITY CORRELATION

$$\mu_i = a_i + b_i T + c_i T^2 \quad \frac{\text{lbm}}{\text{ft-sec}}$$

Species	a x 10^5	b x 10^7	c x 10^{12}	Temperature Range (°K)
O_2	1.693	0.1496	-0.2276	2,000-10,000
N_2	0.970	0.1613	-0.1916	2,000-10,000
O	1.519	0.1875	-0.2228	2,000-10,000
N	0.253	0.2206	-0.3737	2,000-10,000
O^+	0.0	0.0500	-0.1000	8,000-15,000
N^+	0.0	0.0500	-0.1000	8,000-15,000
e^-	0.0	0.0500	-0.1000	8,000-15,000
C	1.997	0.1772	-0.3378	5,000-10,000
H	0.294	0.0889	-0.0811	4,000-10,000
H_2	-0.079	0.0791	-0.0886	4,000-10,000
CO	2.404	0,1363	-0.2184	4,000- 9,000
C_3	2.019	0.1179	-0.1655	1,000- 5,000
CN	2.404	0.1363	-0.2184	4,000- 9,000
C_2H	2.404	0.1363	-0.2184	4,000- 9,000
C_2H_2	1.396	0.0842	-0.6939	1,000- 5,000
C_3H	2.019	0.1179	-0.1655	1,000- 5,000
C_4H	2.019	0.1179	-0.1655	1,000- 5,000
HCN	1.378	0.0965	-0.0948	1,000- 5,000
C_2	1.931	0.1393	-0.2575	4,000- 9,000
C^+	0.0	0.0500	-0.1000	8,000-15,000

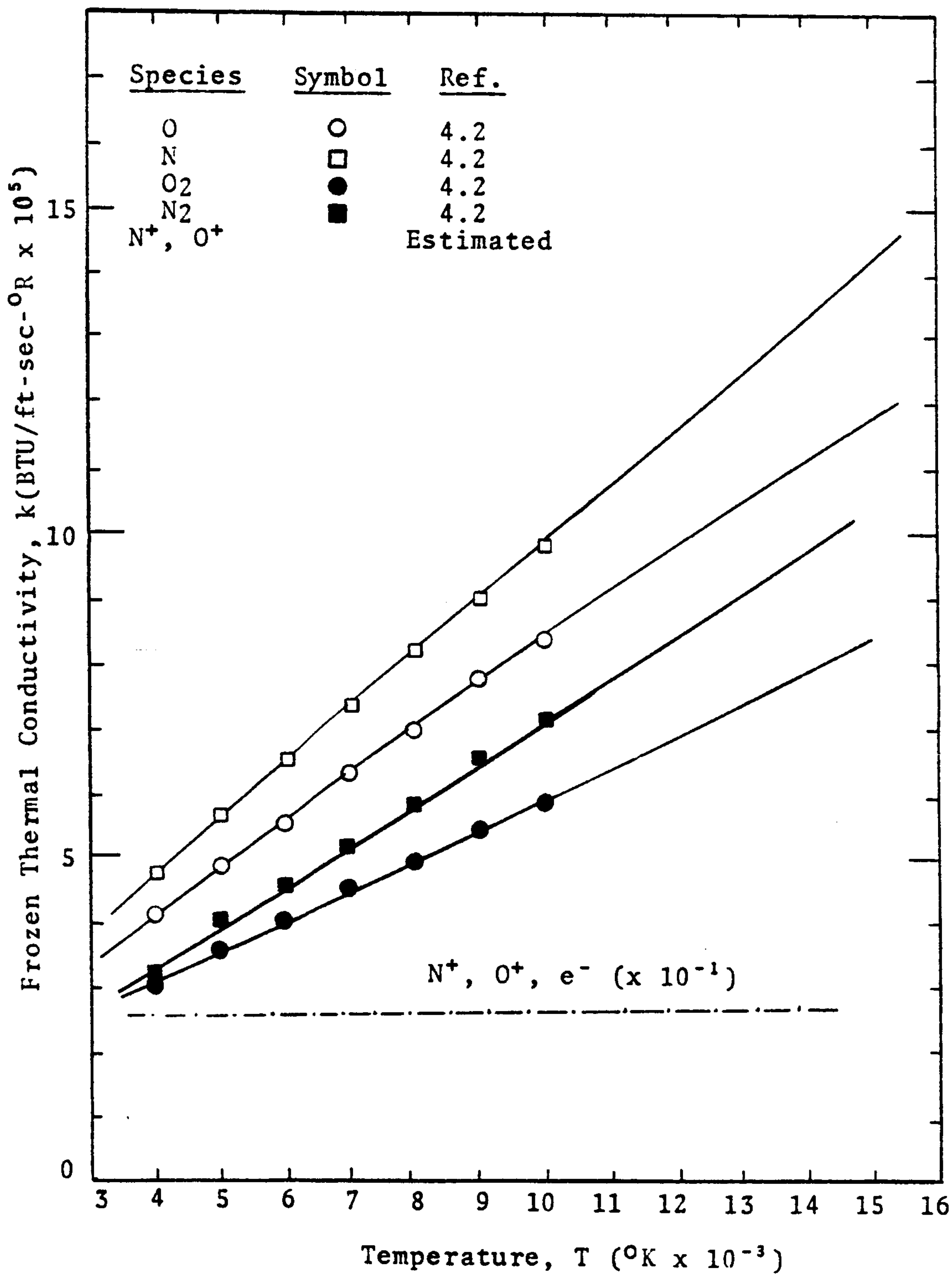


Figure 4.4. Frozen Thermal Conductivity of Air Species at 1 atm.

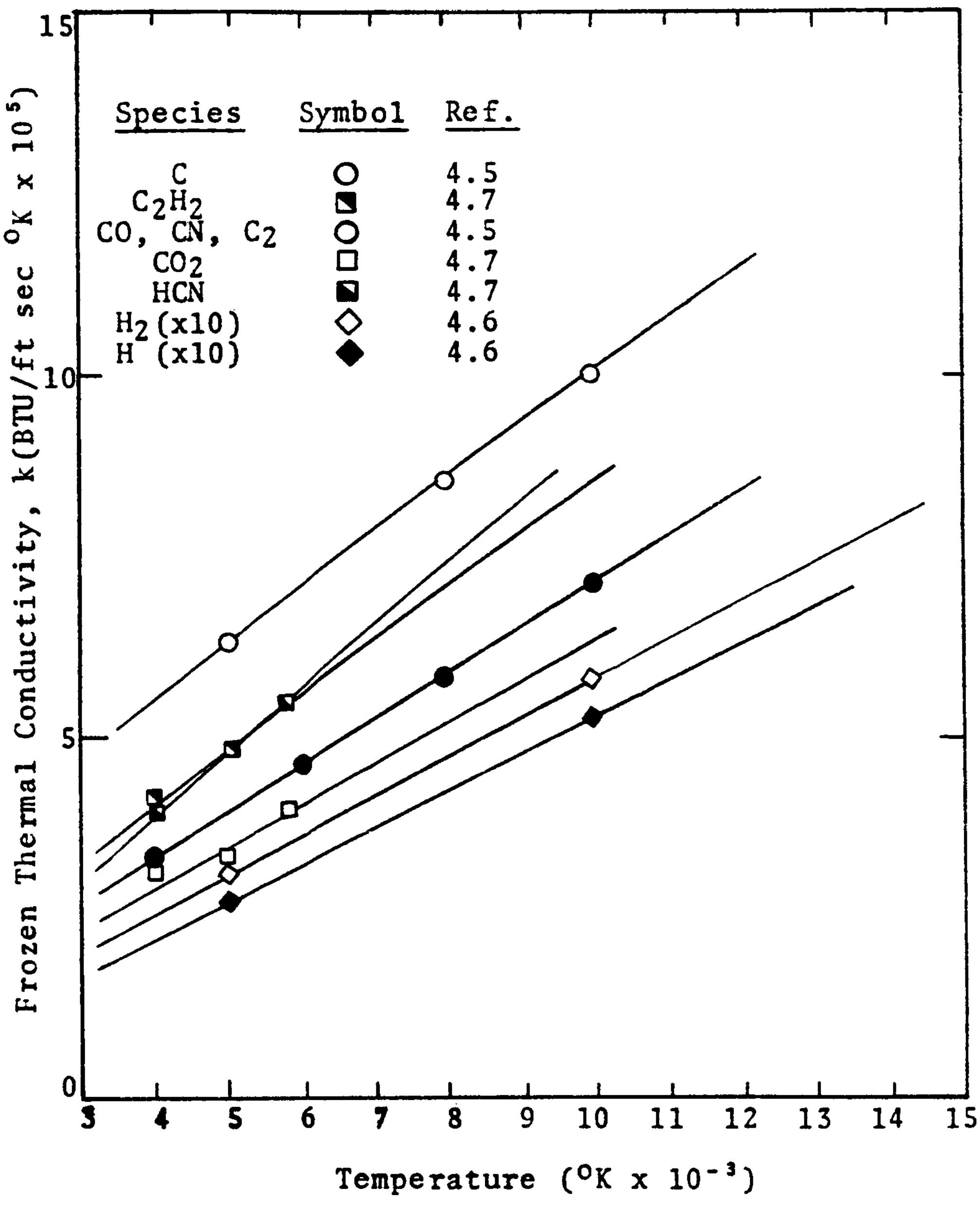


Figure 4.5. Frozen Thermal Conductivity of Ablation Products at 1 atm.

TABLE 4.2

EMPIRICAL CONSTANTS FOR THERMAL CONDUCTIVITY CORRELATION

$k_i = a + bT$ (BTU/ft-sec-°R)

Species	$a \times 10^5$	$b \times 10^2$	Temperature Range (°K)
O_2	1.019	0.4901	2,000-10,000
N_2	0.654	0.6457	2,000-10,000
O	1.250	0.7092	2,000-10,000
N	1.281	0.8593	2,000-10,000
O^+	26.0	0.0	8,000-15,000
N^+	26.0	0.0	8,000-15,000
e^-	26.0	0.0	8,000-15,000
C	2.506	0.7479	5,000-10,000
H	2.496	5.129	4,000-10,000
H_2	3.211	5.344	4,000-10,000
CO	0.859	0.6233	1,000- 5,000
C_3	0.630	0.5804	1,000- 5,000
CN	0.859	0.6233	2,000-10,000
C_2H	1.126	0.7439	1,000- 5,000
C_2H_2	1.126	0.7439	1,000- 5,000
C_3H	0.630	0.5804	1,000- 5,000
C_4H	0.630	0.5804	1,000- 5,000
HCN	0.486	0.8714	1,000- 5,000
C_2	0.859	0.6233	1,000- 5,000
C^+	26.0	0.0	8,000-15,000

where k_f is the frozen mixture thermal conductivity and Φ_{ij} is defined by Equation 4.3. The predicted results of this relationship are given in Figure 4.6 and are compared with the more rigorous predictions.

As shown in Appendix A, the total thermal conductivity is written as:

$$k = k_f + k_r \qquad (4.6)$$

where k_f is given by Equation 4.5 and k_r is given by the following relationship:

$$k_r = \rho \sum_{i=1}^{\nu} D_i h_i \frac{\partial C_i}{\partial T} \qquad (4.7)$$

For binary diffusion, Equation 4.7 can be written as

$$k_r = \rho \mathcal{D}_{12} \sum_{i=1}^{\nu} h_i \frac{\partial C_i}{\partial T} \qquad (4.8)$$

Experimental measurements of a pure nitrogen system have shown that the results of Yos (Ref. 4.7) may be somewhat low for the prediction of the total conductivity of high temperature air.* The comparison

*This discrepancy occurs in the calculation of the reacting thermal conductivity (k_r) and does not reflect upon the accuracy of the theoretical predictions of μ and k_f in Reference 4.7.

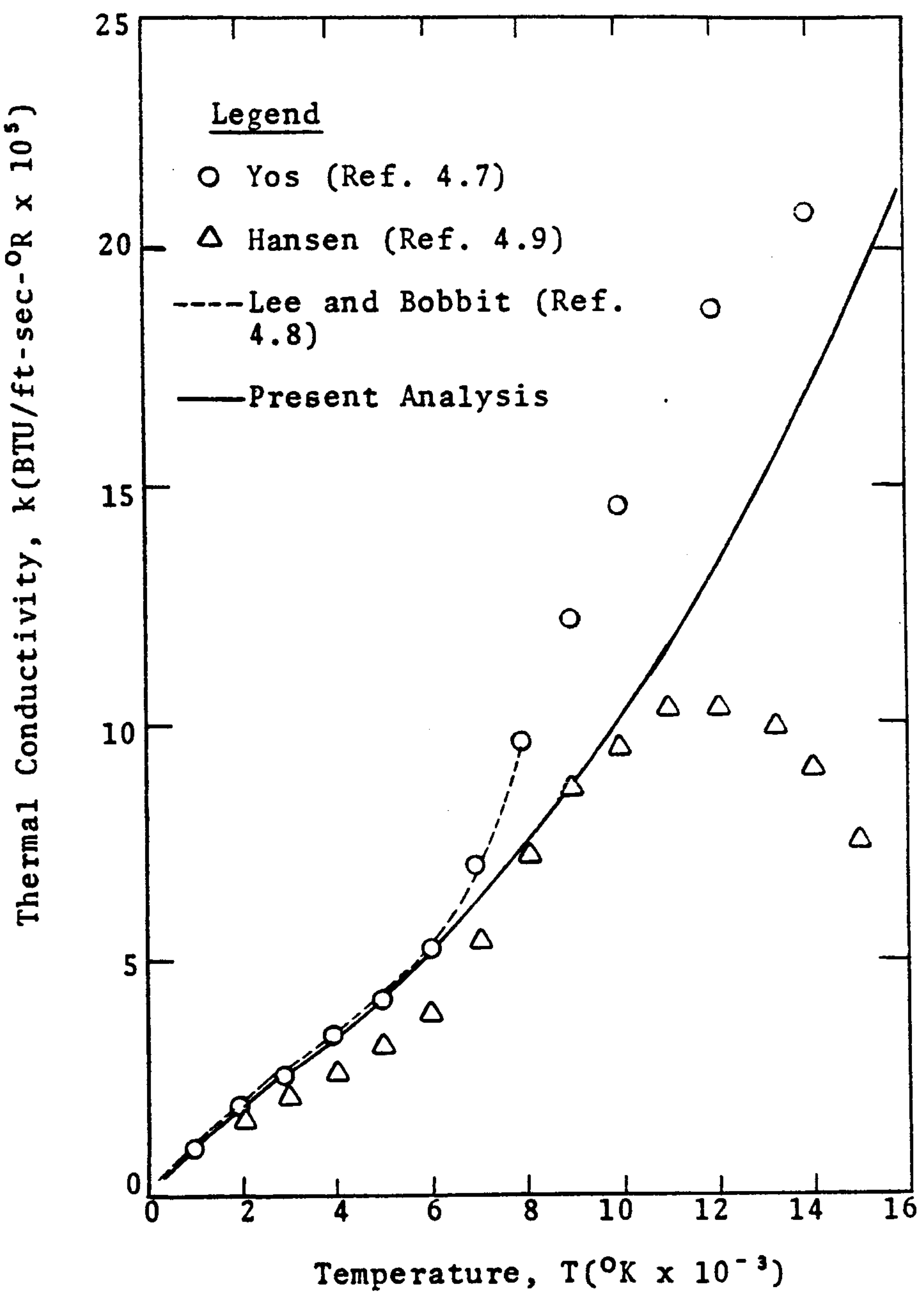


Figure 4.6. Comparison of Predictions for Frozen Thermal Conductivity of Air at 1 atm.

which includes also the results of Hansen (Ref. 4.9) is given in Figure 4.7. Upon considering the results of Figure 4.7, it was decided that an intermediate profile of total thermal conductivity would be estimated. This result was accomplished by assuming a binary diffusion coefficient, $\mathcal{D}_{12}$, given by the following relationship,

$$\mathcal{D}_{12} = \frac{AT^{1.659}}{P} \quad \text{cm}^2/\text{sec} \tag{4.9}$$

where

$$A = 1.22 \times 10^{-5} + 3.11 \times 10^{-9} T \tag{4.10}$$

The constants employed in Equation 4.10 were determined from the predicted thermal conductivity values of Lee and Bobbitt (Ref. 4.8) for temperatures less than 8000°K. These constants were then used for the higher temperature predictions. The results of this correlation are given in Figure 4.8.

<u>Binary Diffusion Coefficients:</u> In view of the multiplicity of binary interactions required it was decided that the following Chapman-Enskog equation for the prediction of this property would be used (Ref. 4.11):

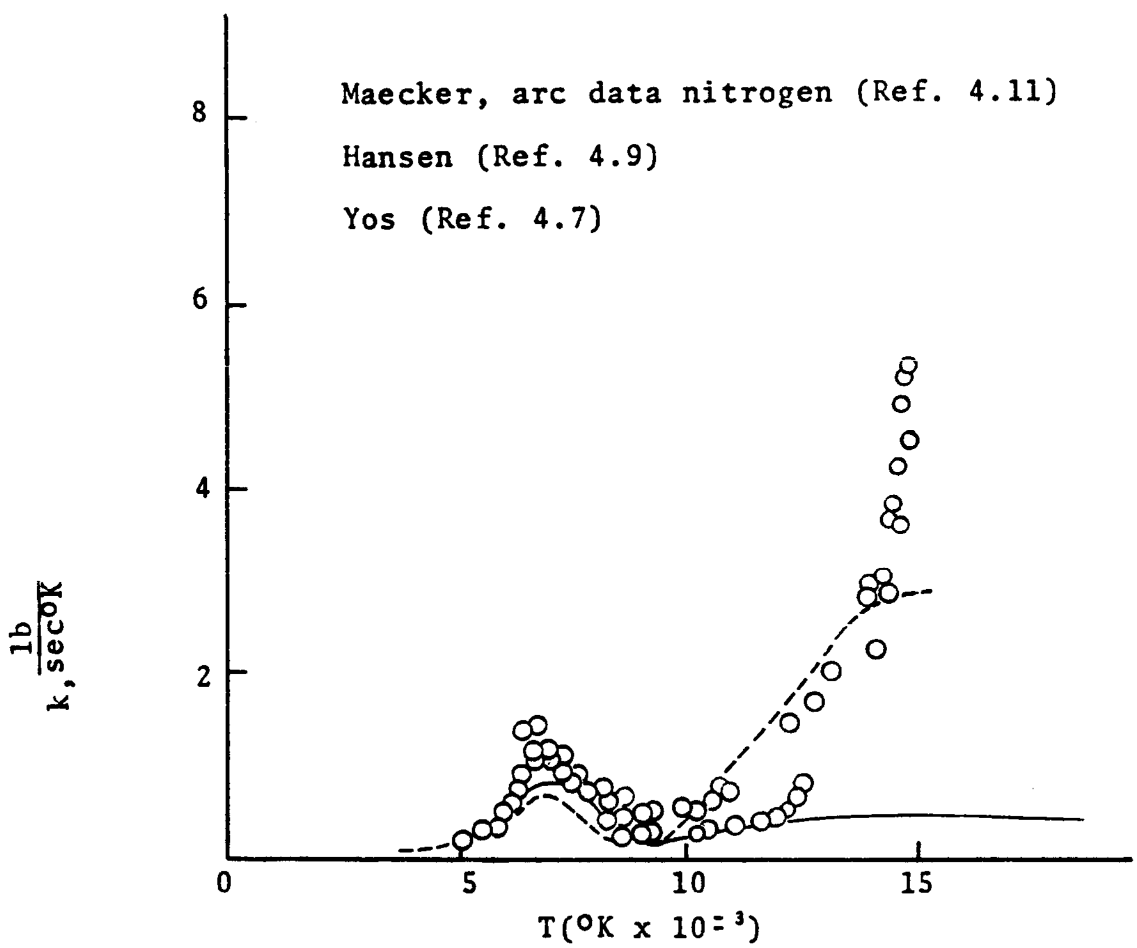


Figure 4.7. Total Thermal Conductivity of Air at One Atmosphere.

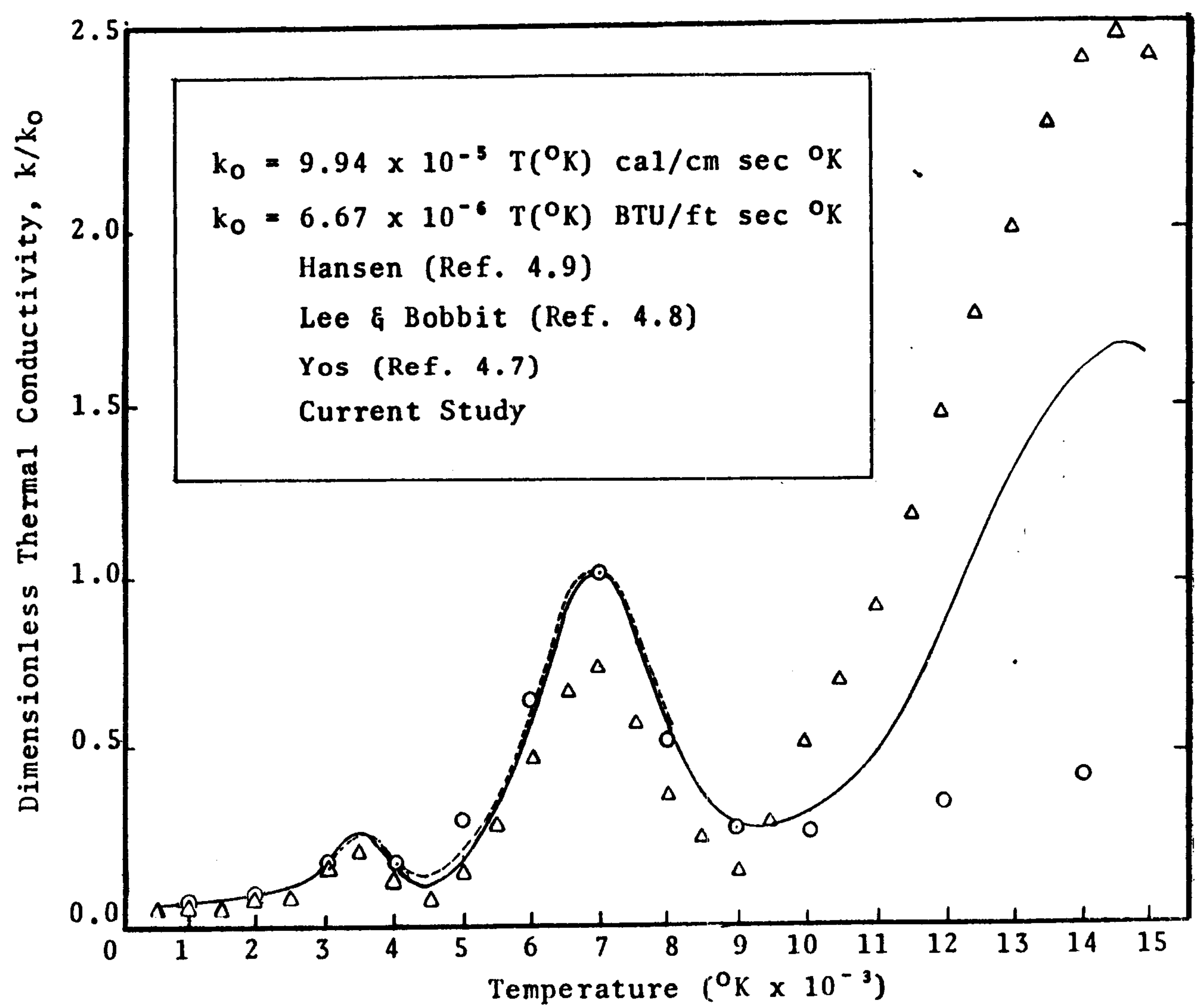


Figure 4.8. Comparison of Several Predictions of the Reacting Thermal Conductivity of Air at 1.0 Atmosphere Pressure.

$$\mathcal{D}_{ij} = 28.28 \times 10^{-7}\, T^{3/2}\left(\frac{M_i+M_j}{2M_iM_j}\right)^{1/2} / P\sigma_{ij}^2\Omega_{ij}^{(1,1)}\ \text{ft}^2/\text{sec} \tag{4.11}$$

where $\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$, the quantities σ_i and σ_j being the collision diameters of the interacting species. The quantity, $\Omega_{ij}^{(1,1)}$ is the Lennard-Jones collision integral for diffusion as determined by the following empirical equation,

$$\Omega_{i,j}^{(1,1)} = 1.061\ (T_{ij}^*)^{-1.56} \tag{4.12}$$

These constants were obtained from a curve-fit of the Lennard-Jones potential as reported by Hirschfelder in Reference 4.11 for $10 \leq T_{ij}^* \leq 1000$ which includes all species and temperatures considered in the current study. The quantity T_{ij}^* is computed as follows,

$$T_{ij}^* = \frac{T}{\varepsilon_{ij}/k_c} \tag{4.13}$$

where $\varepsilon_{ij} = \sqrt{\varepsilon_i\varepsilon_j}$, ε_i and ε_j being the characteristic interaction energies of species i and j.

Values for the collision parameters, σ_i and ε_{i/k_c}, for O_2, N_2, C, H, H_2, CO, CN, C_2H_2, HCN, and C_2, were obtained from Svehla (Ref. 4.5). Since no data was available for C_3, C_2H, C_3H, and C_4H, it was necessary to develop correlations based upon similar species. In Appendix C, the following correlations structure are developed for the prediction of the collision parameters of the above light hydrocarbon species.

Collision Diameter:

$$\sigma_i = 2.69 + 0.0514 \ M_i \tag{4.14}$$

Interaction Energy (C_n molecules):

$$\varepsilon_{i/k} = - 17.0 + 4.02 \ M_i \tag{4.15}$$

Interaction Energy (C_nH_n molecules):

$$\varepsilon_{i/k_c} = - 105. + 12.4 \ M_i \tag{4.16}$$

The collision parameters O, N, O^+, N^+ and e^- were estimated from the theoretically determined binary diffusion coefficients reported by Yun, Wiessman, and Mason (Ref. 4.2) and by Yos (Ref. 4.7). The method of estimating these parameters from the rigorously determined theoretical data is also given in Appendix C.

The behavior of C^+ was then assumed to be similar to that of N^+. A summary of the collision parameters employed in the present study is given in Table 4.3.

Thermodynamic Properties

Thermodynamic data is widely available (Refs. 4.12-4.17) for many substances relative to their values at absolute zero. Generally this data appears in the form of the thermodynamic functions, $(H_T{}^o - H_0{}^o)/RT$ and $(F_T{}^o - H_0{}^o)/RT$ where the superscript (^{o}) denotes the quantity at standard state (the pure component at one atmosphere pressure). The properties $H_T{}^o$ and $F_T{}^o$ computed from these functions will hereafter be referred to as "standard" properties. In the discussion to follow the required polynomial forms for curve-fits of this data are derived.

At constant pressure the following thermodynamic relations exist:

$$dH^o = C_p{}^o \, dT \tag{4.17}$$

$$dS^o = \frac{C_p{}^o \, dT}{T} \tag{4.18}$$

TABLE 4.3

COLLISION PARAMETERS EMPLOYED IN THE CURRENT STUDY

Species	M_i	σ_i	ε_i/k
O_2	32.000	3.467	106.7
N_2	28.016	3.798	71.4
O	16.000	7.990	106.7
N	14.008	7.940	71.4
O^+	16.000	14.220	106.7
N^+	14.008	14.930	71.4
e^-	5.486×10^{-4}	14.930	71.4
C	12.001	3.385	30.6
H	1.008	2.708	37.0
H_2	2.016	2.827	59.7
C_3	36.033	4.450	128.0
CN	26.019	3.856	75.0
C_2H	25.030	3.880	205.0
C_2H_2	26.038	4.033	231.8
C_3H	37.041	4.600	356.0
C_6H	49.052	5.210	504.0
HCN	27.027	3.630	469.1
C_2	24.022	3.913	78.8
C^+	12.011	15.000	30.6

Standard heat capacity data can be conveniently fitted to the following polynomial form:

$$C_p^{\,o} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \qquad (4.19)$$

Substituting this relation into Equation 4.18 and integrating gives:

$$S_T^{\,o} = a_1, \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7 \qquad (4.20)$$

where a_7 is an integration constant. The use of the indefinite integral here is necessary since the polynomial formulation yields an indeterminant expression at absolute zero; however, this does not present any difficulties at temperatures other than absolute zero.

The derivative of the standard free energy of a substance can be defined in terms of standard enthalpy and entropy as

$$dF^o = dH^o - d(TS^o) = dH^o - Tds^o - s_T^o dT \qquad (4.21)$$

From Equations 4.17 and 4.18 it is noted

$$dH^o = TdS^o \qquad (4.22)$$

therefore

$$dF^{o} = - S_T^{o}\ dT \tag{4.28}$$

Integrating this expression in temperature from absolute zero with S_T^{o} defined by Equation 4.20 yields the following,

$$F_T^{o} - F_0^{o} = [a_1(\ln T - 1)T + \frac{a_2T^2}{2} + \frac{a_3T^3}{3} + \frac{a_4T^4}{4} + \frac{a_5T^5}{5} + a_7T] \tag{4.24}$$

In general, standard free energy data is tabulated in non-dimensional form. Performing this nondimensionalization with the quantity $\mathbb{R}T$ and noting that $F_0^{o} = H_0^{o}$ gives

$$\frac{F_T^{o} - H_0^{o}}{\mathbb{R}T} = A_1(1-\ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 - A_7 \tag{4.25}$$

where $A_1 = a_1/\mathbb{R}$, $a_2 = a_2/\mathbb{R}, \ldots$, $A_5 = a_5/\mathbb{R}$ and $A_7 = a_7/\mathbb{R}$. From Equations 4.17 and 4.18 the comparable polynomial expression for standard enthalpy can be derived.

$$\frac{H_T^{o} - H_0^{o}}{\mathbb{R}T} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 \tag{4.26}$$

We have thus derived polynomial expressions for the thermodynamic functions of standard, heat capacity, entropy, enthalpy, and free energy relative to $0^{o}K$. In order to determine absolute values of enthalpy and free energy from these functions it is necessary to specify a reference state from which the enthalpy (and free energy) at absolute zero can be determined. It is convenient to select the elements at $298.16^{o}K$ and one atmosphere pressure for the reference state, since this is widely used.

The reference state is established by defining the absolute enthalpy (H_T^o) of the elements equal to zero at $298.16^{o}K$. The enthalpy of an element at absolute zero (H_0^o) is then equal to the change in enthalpy from the reference temperature to absolute zero, or simply $(H^o_{298.16} - H_0^o)$. For a compound the absolute enthalpy at the reference temperature is no longer equal to zero, but is equal to the heat of formation of the particular compound from the reference elements. Therefore, in order to determine the enthalpy of a compound at absolute zero from the tabulated enthalpy function it is necessary to correct for the heat of formation:

$$H_0^o = -(H^o_{298.16} - H_0^o) + (\Delta H_f)_{298.16} \qquad (4.27)$$

where the quantity, $(H^o_{298.16} - H_0^o)$ is available from the tabulated values of the enthalpy function. In non-dimensional form, this equation becomes

$$\frac{H_0^o}{\mathbb{R}T} = \frac{(\Delta H_f)_{298.16} - (H^o_{298.16} \; H_0^o)}{\mathbb{R}T} \tag{4.28}$$

Having defined a reference state, it is a simple matter to determine the thermodynamic properties from the thermodynamic functions as follows:

$$\frac{F_T^o}{\mathbb{R}T} = A_1 \; (1 - \ln T) - \frac{A_2}{2} - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7 \tag{4.29}$$

$$\frac{H_T^o}{\mathbb{R}T} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \tag{4.30}$$

where

$$A_6 = H_0^o/\mathbb{R} = [(\Delta H_f)_{298.16} - (H^o_{298.16} - H_0^o)] \; \mathbb{R} \tag{4.31}$$

Thermodynamic data for the species of interest were fitted to the previously discussed polynomials by the method described in Appendix D. The resulting coefficients ($A_1, A_2, \ldots A_7$) give predictions of free energy and enthalpy which reproduced the theoretical data to four significant figures. The maximum error in the entropy and heat capacity correlation was 2.12%. To further test the applicability of these results a free minimization technique,* using these correlations, was performed to determine the compositions which were then used with the enthalpy correlation to predict the total heat capacity of air by the following equation:

$$C_p = \sum Y_i C^o_{p_i} + \sum H_i \frac{\partial Y_i}{\partial T} \tag{4.32}$$

The predicted results were then compared with those of other investigators as shown in Figure 4.9. Excellent agreement was obtained.

Radiation Properties

The radiative flux divergence (dq_R/dy) appearing in Equation 3.6 is defined as follows (Ref. 4.20):

$$\frac{dq_R}{dy} = \int_0^{\infty} \int_0^{4\pi} \alpha(y,\nu)\,[B(y,\nu) - I(y,\nu,\Omega)]\, d\Omega d\nu \tag{4.33}$$

where q_R = the radiative flux in the normal direction from the body,

$\alpha(y,\nu)$ = volumetric absorption coefficient,

*Described in Appendix E.

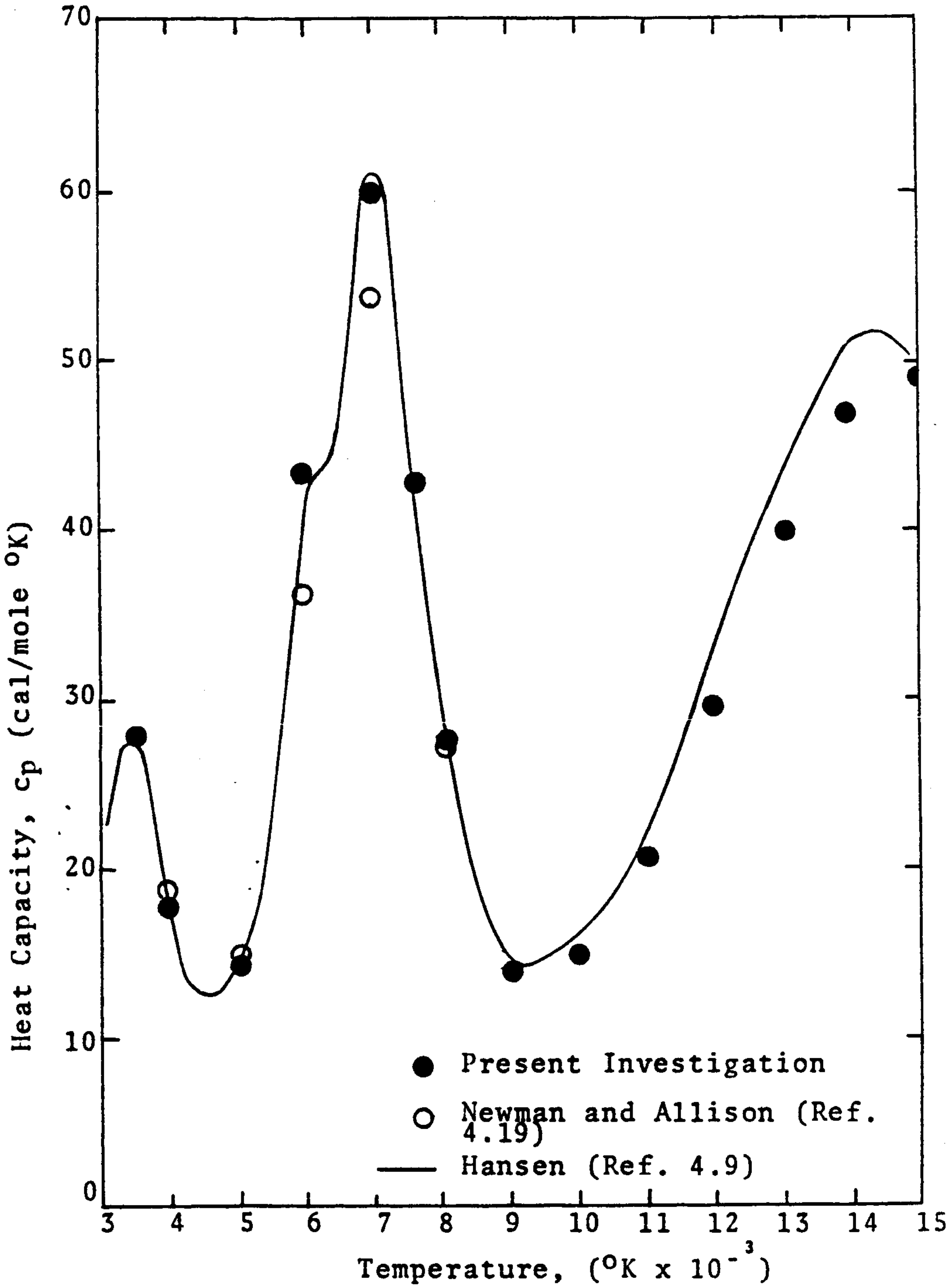


Figure 4.9. Comparison of Mixture Reacting Heat Capacity for Air and One Atmosphere.

$B(y,\nu)$ = Plankian radiation intensity,

$I(y,\nu,\Omega)$ = radiation intensity,

$d\Omega$ = solid angle about the unit vector $\bar{\Omega}$,

ν = frequency.

Given temperature and species distributions, the above integral can be evaluated theoretically. However, due to the discontinuous nature of the absorption coefficients numerical integration, in practice, is a formidable task. Typical absorption coefficient distributions are given in Figures 4.10 and 4.11 to illustrate the extent of this adversity (Ref. 4.24).

To overcome the numerical difficulties associated with the integration of distributions such as those given in Figures 4.10 and 4.11, the frequency range is arbitrarily sub-divided into regions (bands) with which the discontinuous variations are averaged. Continuum radiation bands are used to represent wider regions of continuous radiation while line bands are used to model the effects of the various discontinuous (line) contributions (see Figures 4.10 and 4.11). As in the numerical integration of continuous functions, the use of more bands leads to more accurate representation of the radiative process. In developing radiation models for computer implementation, some compromise must be made between the execution time and the number of bands.

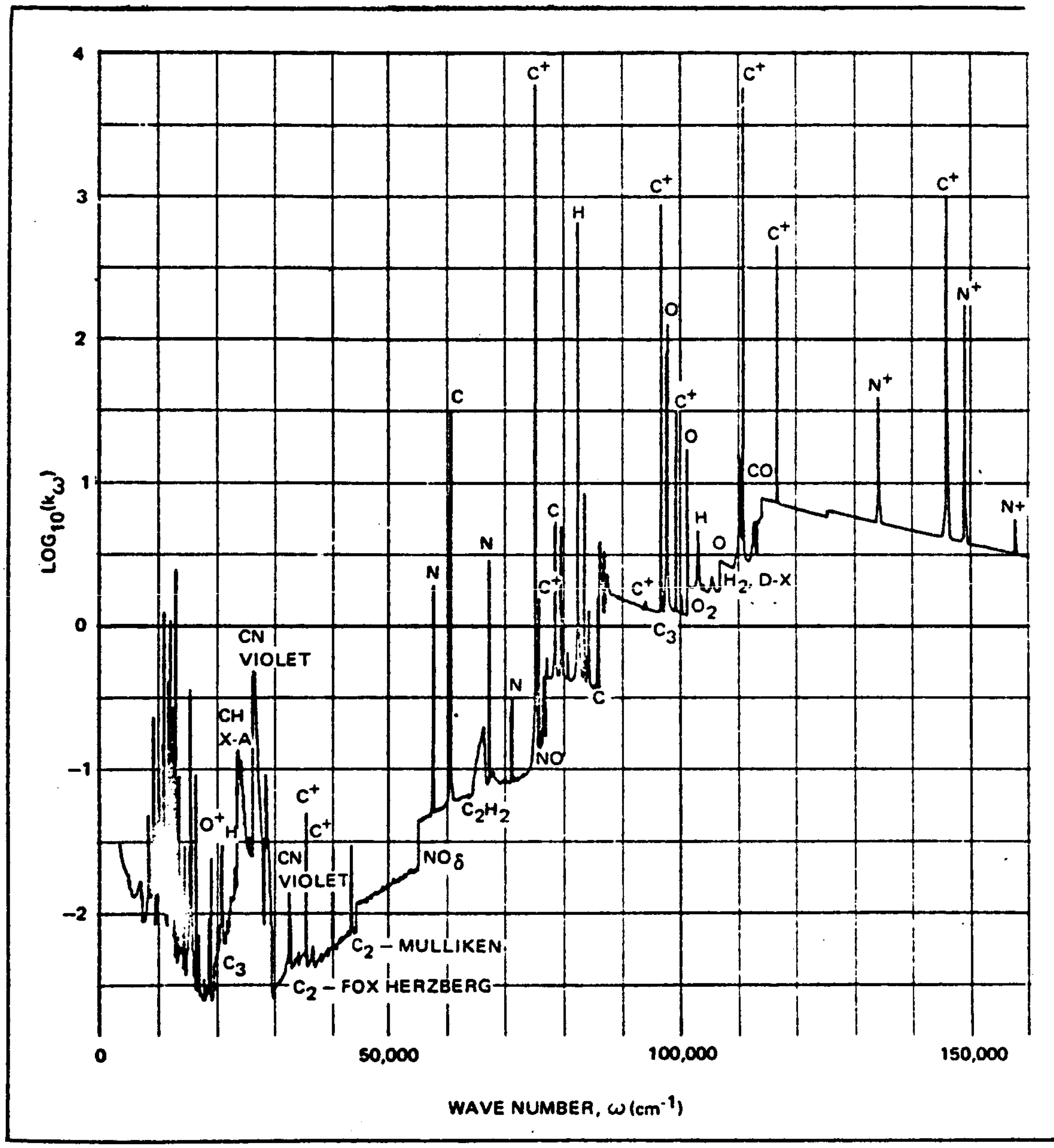
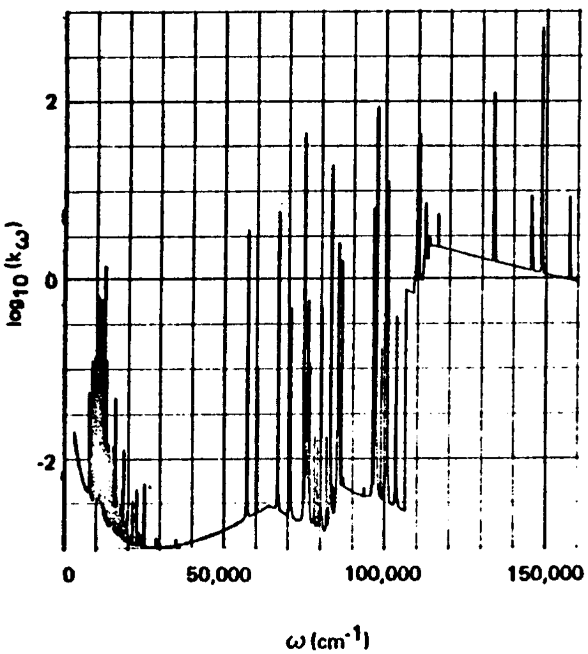
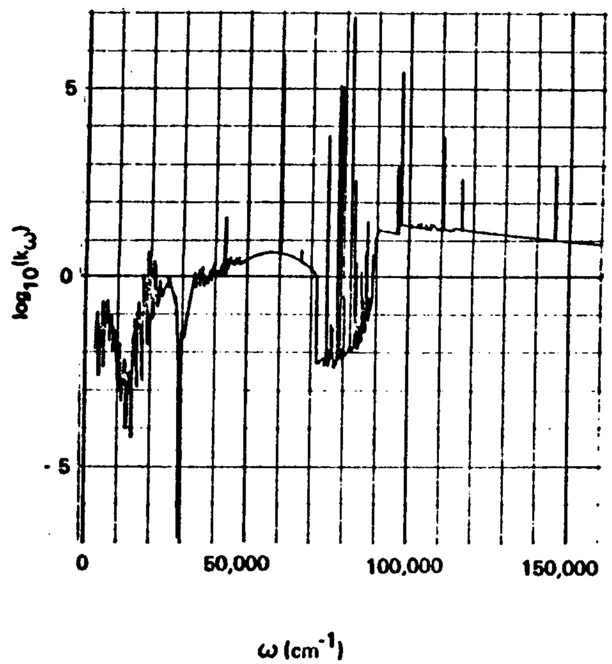


Figure 4.10. Spectral Absorption Coefficient of Air-Carbon Phenolic Ablation Products Mixture for P = 1 and T = 16,000°K (Ref. 4.24).



T = 15,000°K, C_A = 0



T = 5,000°K, C_A = 1.0

Figure 4.11. Typical Variation of k_ω Across the Shock Layer with Ablation Productions Injection (Ref. 4.24).

The radiation model used in the present work is a revision (Engel, Ref. 4.21) of a coupled line and continuum model originally developed by Wilson (Ref. 4.20). The program (LRAD3) provides a useful tool for evaluating the radiation flux and the radiative flux divergence across a slab of gas containing both air and ablation species.

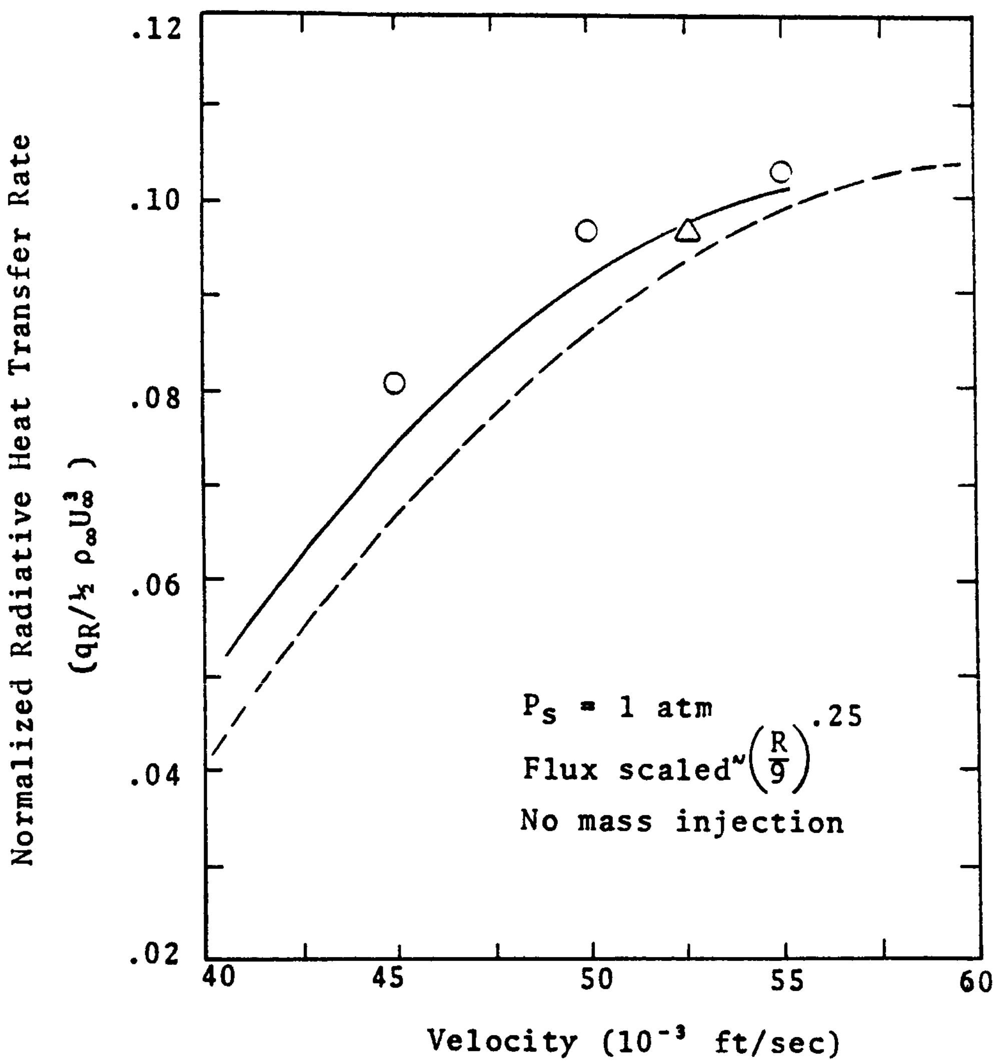
The existing program contains twelve continuum frequency bands and nine line bands. A comparison with a more detailed model (RATRAP) in Reference 4.22, revealed that the existing analysis predicted total heat flux values within 5%. The following species are considered in the program used in the current study.

$$\left.\begin{array}{l} C \\ H \\ N \\ O \end{array}\right\} \text{Continuum and Lines} \qquad \left.\begin{array}{l} CO \\ C_2 \\ C_3 \\ O_2 \\ H_2 \\ N_2 \\ C_2H \\ e^- \end{array}\right\} \text{Continuum}$$

The program LRAD 3 was included in reduced form (air species only) in a program called VISRAD I which was developed by Spradley and Engel (Ref. 4.23). Figure 4.12 presents a comparison of dimensionless radiative heating rates as a function of free-stream velocity by several investigators. For this no mass injection case the comparison is quite reasonable. All investigators reported on this figure have line and continuum radiation calculations for air at stagnation line. Although this case does not contain the effects of ablation species, it is a standard for comparison of computational techniques.

Summary

Through the development of correlations from rigorously determined theoretical data an efficient means of predicting the high temperature transport and thermodynamic properties of ablation products and air species has been established. In so doing, the theoretically accurate properties can be well approximated without resorting to the more rigorous calculation procedures normally required for their prediction. These estimates are of course limited to the capabilities of the rigorous theoretical predictions. But, in the absence of sufficient experimental data, the rigorous



○ Rigdon, et al. (July, 1969) (Ref. 4.24).
---Page, et al. (Ref. 4.25).
△ Wilson (April, 1969) (Ref. 4.20).
——Present results (with Wilson's Radiation Model).

Figure 4.12. Comparison of Dimensionless Radiative Heating Rates (Ref. 4.21).

theoretical predictions as well as the correlations presented in this chapter represent the best available means of predicting transport and thermodynamic properties of the reacting gas mixtures encountered in the radiative heating of entry vehicles.

Finally, the radiative transport model employed in this study has shown excellent agreement with the predictions of models employed by other investigators and represents a well-balanced compromise between accuracy and computational convenience.

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CHAPTER V

NUMERICAL IMPLEMENTATION OF THIN SHOCK LAYER EQUATIONS

Introduction

In the previous chapters the thin shock layer equations have been developed in a form which is convenient for numerical implementation. In addition, convenient models have been developed for predictions of the necessary thermodynamic, transport, and radiative properties. This chapter will consist of a detailed description of the numerical implementation of the previously developed flowfield equations and property models to obtain a fully coupled analysis of stagnation region heating of ablative thermal protection systems.

The method of presentation will be to first outline the overall analysis with a general description of the logical process. Secondly, each of the major subprograms related to the numerical solution of the conservation equations will be separately discussed in detail. The discussion will then be concluded with a review of the computational experience with the overall analysis.

Coupled Stagnation Line Analysis With Binary Diffusion

A simplified flow diagram of the overall stagnation line analysis (SLAB)*,** as developed in this study is given in Figure 5.1. The major input data consist of free-stream velocity (U_∞), a free-stream density (ρ_∞), body radius (R), wall temperature (T_W), and mass injection rate (RVW), initial estimates of T, ρ, and $\rho\mu$ profiles and the transformed shock standoff distance $\tilde{\delta}$.* Also included are initial estimates of the injected gas compositions which have elemental ratios consistent with the selected ablator. The initialization phase consists primarily of determining the shock temperature (T_S), the normal velocity at the shock (v_S) and the pressure (P_S) from the Rankine-Hugoniot Equations (Eqs. 3.81-3.84) using the specified values of free-stream velocity (U_∞) and density (ρ_∞).

From the specified ρ and $\rho\mu$ profiles and the specified, transformed stand-off distance $\tilde{\delta}$, the momentum equation (Eq. 3.99) is solved to obtain an estimate of the velocity profile (MOMTM). Using the computed velocity profile and the assumed temperature and density profiles, the elemental continuity equations (Eq. 3.88) are then solved (ELEMNT). The chemical equilibrium calculation (CHEMEQ) is then performed to determine the species

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*A more detailed description of these and other input parameters is given in Appendix F.

**Developed in collaboration with C. D. Engel (Ref. 5.6).

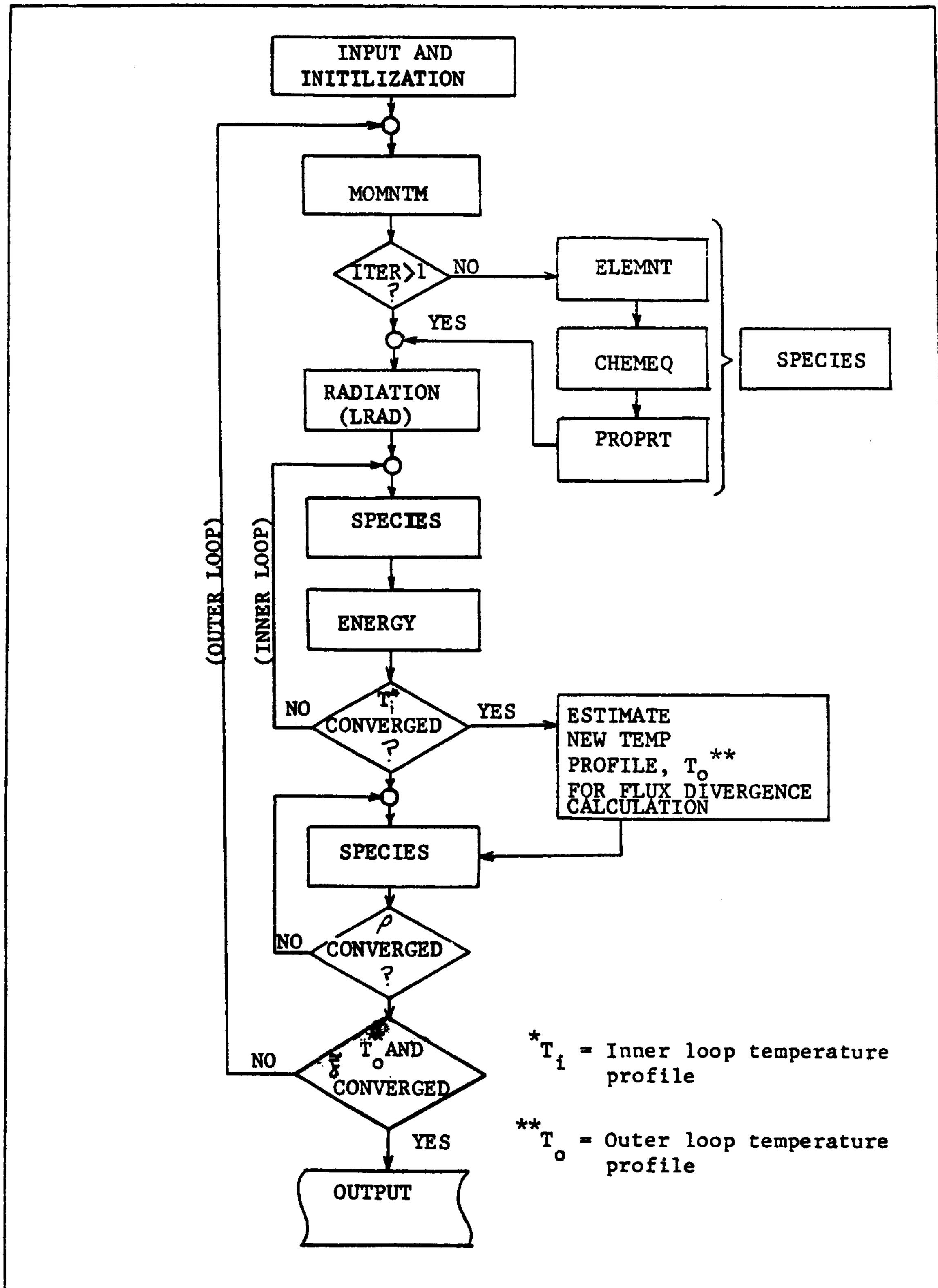

Figure 5.1. Simplified Flow Diagram for Stagnation Line Heating Analysis with Binary Diffusion (SLAB).

composition profiles. The reacting gas properties are then determined (PROPRT) along with the radiative flux divergence ($dq_R/d\eta$) from LRAD. From the flux divergence and the gas properties, the temperature profile is determined (ENERGY). The computed temperature profile is used with the previous density and velocity profiles to obtain revised thermodynamic and transport property distributions which are in turn used to compute a new temperature profile. This process is repeated until convergence is achieved. From the final temperature profile and the initial temperature profile (on which the radiative flux divergence was based), a new profile is estimated for the next cycle through the outer loop (See Figure 5.1). The density profile is then updated to correspond to the revised temperature distribution and the last computed velocity distribution. The outer loop is repeated until the momentum and energy solutions and the shock standoff distance have simultaneously converged.

Numerical Solution of the Conservation Equations: The basic conservation equations (Eqs. 3.97, 3.99 and 3.100) can be reduced to the form:

$$\frac{d^2W}{d\eta^2} + a_1 \frac{dW}{d\eta} + a_2 W = a_3 \qquad (5.1)$$

Using three point, variable step size, finite-difference approximation at (s-2)* points across the flowfield, the numerical form of the equations becomes

$$\bar{\bar{A}} \cdot \bar{W} = \bar{B}$$

where $\bar{\bar{A}}$ is a tridiagonal matrix of order (s-2). This form lends itself to numerical solution by a tridiagonal matrix inversion algorithm (Ref. 5.1). The specific treatment of the basic conservation equations is the subject of the following discussion.

<u>Elemental Continuity Equations</u>: Assuming binary diffusion, the elemental continuity equations (Eqs. 3.97) can be expressed in the following form,

$$\frac{d^2 C_j}{d\eta^2} + a_1 \frac{dC_j}{d\eta} = 0 \qquad j=1, 2, \ldots \ell \tag{5.3}$$

where

$$a_1 = 2\frac{d\ln\rho}{d\eta} + \frac{d\ln\rho\mathcal{D}_{12}}{d\eta} - \frac{v\tilde{\delta}}{\rho\mathcal{D}_{12}} \tag{5.4}$$

The shock boundary conditions (of the first kind) for the elemental continuity equations are the elemental composition of air ($C_{N,s} = 0.774$ and $C_{O,s} = 0.226$).

*Point 1 is at the wall and point s is at the shock. Finite differencing is required only at the intermediate points, since the extreme values established as boundary conditions.

The boundary conditions at the wall can be obtained from Equations 3.59 as follows:

$$\rho v \tilde{C}_j^{+} + \tilde{J}_j^{+} = \rho v \tilde{C}_j^{-} + \tilde{J}_j^{-} = \tilde{I}_j = \begin{bmatrix}\text{total mass flux} \\ \text{of element j at} \\ \text{the wall}\end{bmatrix} \tag{5.5}$$

where the quantity I_j is determined from the product of the elemental composition of the ablator ($\tilde{C}_j^{-}$) and the mass injection rate (ρv) wall. Assuming binary diffusion:*

$$\tilde{J}_j = - \frac{\rho^2 \mathscr{D}_{12}}{\tilde{\delta}} \frac{dC_j}{d\eta} \tag{5.6}$$

Equation 5.5 can be written as

$$\rho v \tilde{C}_j - \rho^2 \frac{\mathscr{D}_{12}}{\tilde{\delta}} \frac{d\tilde{C}_j}{d\eta} = \tilde{I}_j \tag{5.7}$$

A boundary condition of the third kind is thus obtained for each of the elemental continuity equations. The treatment of this type of boundary condition will be subsequently discussed.

The binary diffusion coefficient appearing in the previous equations is determined from the following form of the Chapman-Enskog Equation (Eq. 2.32),

$$\mathscr{D}_{12} = A\ T^{1.656}/P \qquad (\text{ft}^2/\text{sec}) \tag{5.8}$$

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*Equation 5.6 is obtained from the Dorodnitzn transformation of Equation 3.23.

where,

$$A = \frac{26.65 \times 10^{-7} \sqrt{\dfrac{M_i + M_j}{2M_iM_j}}}{\sigma_{ij}^2 \, (\varepsilon_{ij}/k_c)^{0.156}}$$

The quantity A, which is independent of temperature and pressure, is thus defined as the characteristic diffusion parameter, since it is a function only of the selected collision data. Typical elemental composition profiles of carbon as a function of the characteristic diffusion parameter are given in Figure 5.2.

Assuming velocity, density, and temperature profiles, the elemental continuity equation can be solved in the following manner. First, finite-differencing the third order wall boundary condition gives

$$(\rho v C_i)_1 - \left.\frac{\rho^2 \mathcal{D}_{12}}{\tilde{s}}\right|_1 \left(\frac{\tilde{C}_{j,2} - \tilde{C}_{j,1}}{\eta_2 - \eta_1}\right) = \tilde{I}_j \tag{5.9}$$

Rearranging and noting that $\eta_1 = o$ yields

$$B_1 \tilde{C}_{i,1} + C_1 \tilde{C}_{i,2} = \tilde{I}_j \tag{5.10}$$

where

$$B_1 = 1 + \frac{(\rho \mathcal{D}_{12}/v)_1}{\tilde{\delta}\eta_2} \tag{5.11}$$

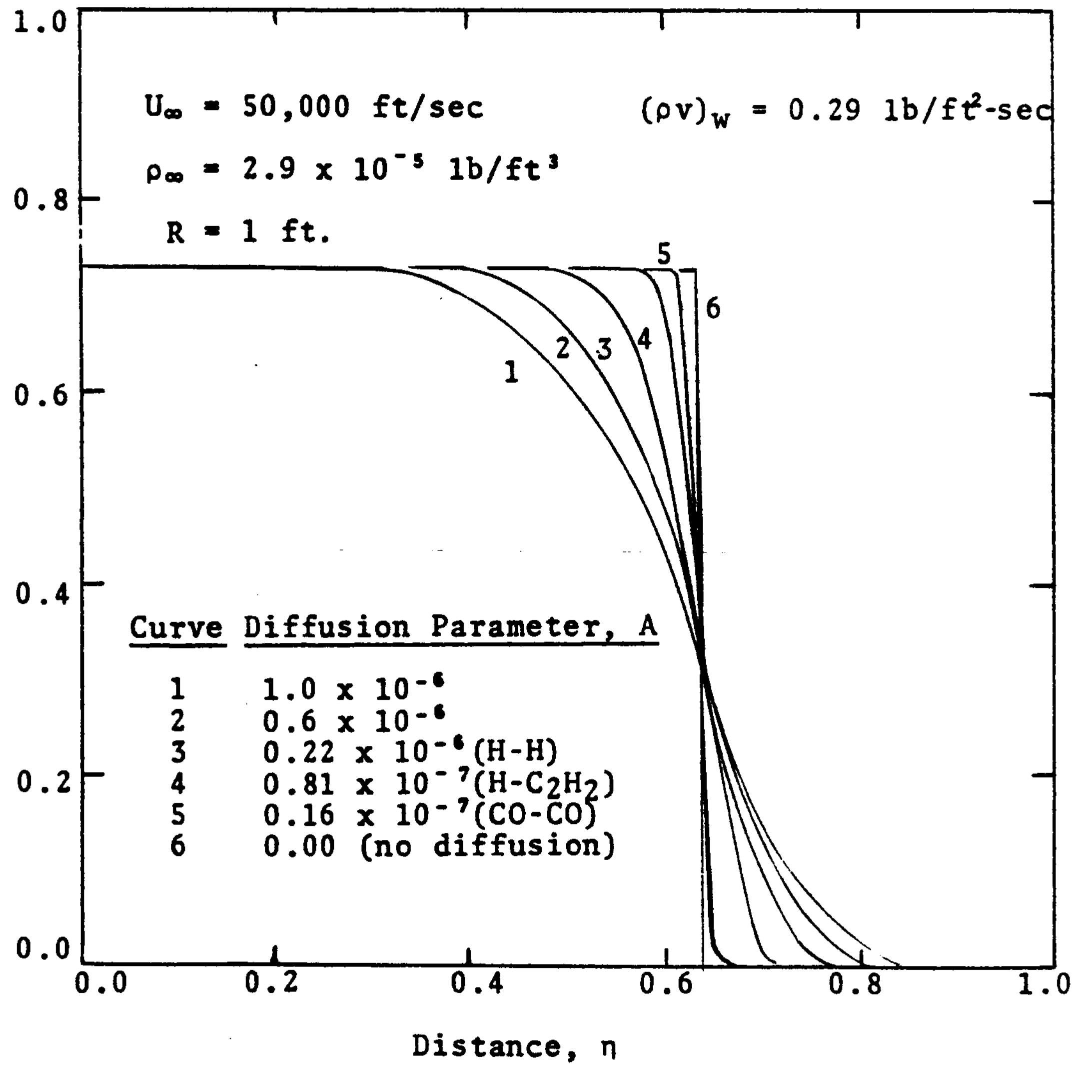

Figure 5.2. Composition Profiles of Elemental Carbon With Various Characteristic Diffusion Parameters.

and

$$C_1 = - \frac{(\rho\mathcal{D}_{12}/v)_1}{\tilde{\delta}\eta_2} \tag{5.12}$$

Equation 5.10 is in a form that will fit into the tridiagonal matrix scheme as will be discussed.

At each subsequent grid point in the flowfield, the derivative terms are then approximated by the following variable step-size finite-difference equations (Ref. 5.8),

$$\left.\frac{dW}{d\eta}\right|_n = F_n^1 W_{n+1} + G_n^1 W_n + H_n^1 W_{n-1} \tag{5.13}$$

and

$$\frac{d^2W}{d\eta^2} = F_n^2 W_{n+1} + G_n^2 W_n + H_n^2 W_{n-1} \tag{5.14}$$

where

$$F_n^1 = \Delta\eta_{n-1}/\Delta\eta_n\,(\Delta\eta_n + \Delta\eta_{n-1}) \tag{5.15}$$

$$G_n^1 = (\Delta\eta_n - \Delta\eta_{n-1})/(\Delta\eta_n\Delta\eta_{n-1}) \tag{5.16}$$

$$H_n^1 = -\Delta\eta_n/\Delta\eta_{n-1}(\Delta\eta_n + \Delta\eta_{n-1}) \tag{5.17}$$

$$F_n^2 = 2/\Delta\eta_n\,(\Delta\eta_n + \Delta\eta_{n-1}) \tag{5.18}$$

$$G_n^2 = -2/\Delta\eta_n\Delta\eta_{n-1} \tag{5.19}$$

$$H_n^2 = 2/\Delta\eta_{n-1}(\Delta\eta_n + \Delta\eta_{n-1}) \tag{5.20}$$

In finite-differenced form, the transformed elemental continuity equations (Eqs. 5.3) thus become

$$(H_n^2 + a_{1,n}H_n^1)\,\tilde{C}_{j,n-1} + (G_n^2 + a_{1,n}G_n^1)\,\tilde{C}_{j,n}$$

$$+ (F_n^2 + a_{1,n}F_n^2)\,\tilde{C}_{j,n+1} = 0 \tag{5.21}$$

which is of the form:

$$A_n\tilde{C}_{j,n-1} + B_n\tilde{C}_{j,n} + C_n\tilde{C}_{j,n+1} = 0$$

Performing this operation at each finite-difference station to n = s-1, yields the following matrix form (see Figure 5.3)

$$\begin{bmatrix} B_1 & C_1 & & & & & \\ A_2 & B_2 & C_2 & & & & \\ & A_3 & B_3 & C_3 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & A_{s-2} & B_{s-2} & C_{s-2} \\ & & & & & A_{s-1} & B_{s-1} \end{bmatrix} \cdot \begin{bmatrix} \tilde{C}_{j,1} \\ \tilde{C}_{j,2} \\ \tilde{C}_{j,3} \\ \cdot \\ \cdot \\ \cdot \\ \tilde{C}_{j,s-2} \\ \tilde{C}_{j,s-1} \end{bmatrix} = \begin{bmatrix} -\tilde{I}_j \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ C_{s-1}\tilde{C}_{j,s} \end{bmatrix} \tag{5.22}$$

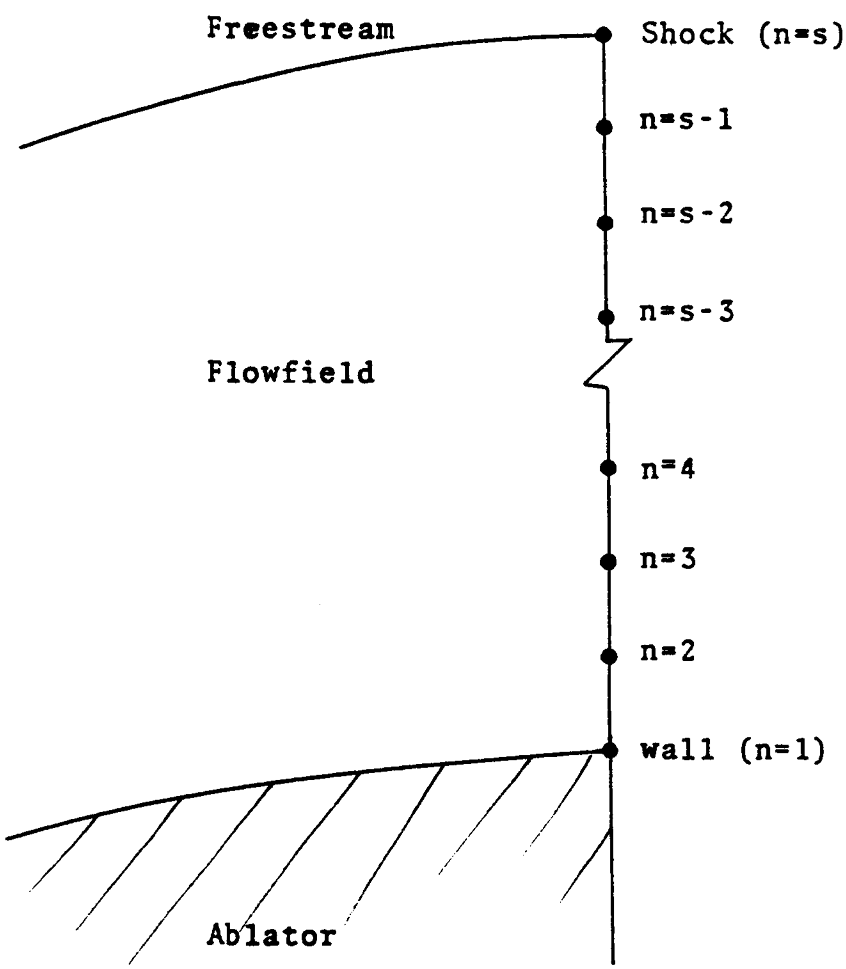

Figure 5.3. Illustration of One-dimensional Finite-difference Network.

Equation 5.22 was solved by the tridiagonal inversion algorithm program given by Conte (Ref. 5.1) and implemented in the Fortran Subprogram TRID appearing in the overall listing given in Appendix F.

The variable stepsize distribution employed in this analysis was determined from the temperature distribution, with the maximum size being $\Delta\eta = 0.04$. Generally, 55-60 steps are generated between $\eta = 0.0$ and $\eta = 1.0$. The convergence of the numerical solution of Equation 5.22 was verified by reducing the stepsize and comparing the resulting solutions. Such a comparison is given in Table 5.1. The maximum difference detected by this comparison was 0.0063. It was therefore concluded that the numerical procedure was convergent. The numerical procedure discussed in this section was implemented in the Fortran subroutine ELEMNT, a listing of which appears in the overall program listing given in Appendix F.

<u>Momentum Equation</u>: The solution of the momentum equation (Eq. 3.99) follows essentially the same procedure as the previously discussed elemental solution. The major difference is that the momentum equation is non-linear. The solution technique, developed by Engel (Ref. 5.2) is given in the following discussion.

TABLE 5.1

COMPARISON OF ELEMENTAL CARBON DISTRIBUTION FOR ETA DISTRIBUTIONS OF 59 AND 126 STEPS

η*	$\tilde{C}_C$ (s = 59)	$\tilde{C}_C$ (s = 126)
0.000	0.6921	0.6909
0.045	0.6762	0.6742
0.080	0.6485	0.6459
0.100	0.6228	0.6199
0.140	0.5410	0.5392
0.180	0.4211	0.4229
0.220	0.2914	0.2977
0.260	0.1859	0.1915
0.300	0.1108	0.1136
0.350	0.0511	0.0517
0.380	0.0290	0.0293
0.440	0.0066	0.0068
0.500	0.0007	0.0009
0.540	0.0001	0.0001
0.560	0.0000	0.0000
1.000	0.0000	0.0000

*Selected points

Integration of Equation 3.95, gives

$$\rho v = -2 \left(\frac{\partial u}{\partial x}\right)_s \tilde{\delta} f \tag{5.23}$$

which can be used to eliminate ρv in the momentum equation (Eq. 3.99). This substitution yields the following third order nonlinear ordinary differential equation,

$$(\rho \mu f'')' + 2 \, Re_s \, \tilde{\delta}^2 \left(\frac{\partial u}{\partial x}\right)_s ff'' +$$

$$\frac{Re_s \, \tilde{\delta}^2}{(\partial u/\partial x)_s} \left[\frac{2\bar{\rho}(1-\bar{\rho})}{\rho} \left(\frac{\partial u}{\partial x}\right)_s^2\right] (f')^2 = 0 \tag{5.24}$$

The boundary conditions for these equations are established in the development to follow. From Equation 3.27 and L'Hospital's rule gives:

$$\lim_{x \to o} f' = \lim_{x \to o} \frac{(\partial u/\partial x)}{(\partial u/\partial x)_s} = \frac{u}{u_s} \tag{5.25}$$

At $x = 0$ and $\eta = 1$, $u = u_s$, therefore $f' = 1$. Similarly, at $x = 0$ and $\eta = 0$, $u = 0$, therefore $f' = 0$. A third boundary condition is obtained by evaluating Equation 5.23 at the wall*

$$f = f_w = \frac{(\rho v)_w}{2\tilde{\delta}} \tag{5.26}$$

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*For a concentric shock, it can be shown from Equation 3.78 that $(\partial u/\partial x)_s = 1$.

The momentum equation (Eq. 5.24) can be reduced to a first and a second order equation by defining

$$\zeta = \frac{f'}{\tilde{\delta}} \tag{5.27}$$

Substitution of Equation 5.27 into 5.24 and noting that $(\partial u/\partial x)_s = 1$ for a concentric shock gives,

$$(\rho\mu)\ \zeta'' + [2\ Re_s\ \tilde{\delta}^2\ f + (\rho\mu)']\ \zeta - Re_s\ \tilde{\delta}^3\ \zeta^2$$

$$= \frac{-2\ Re_s\ \tilde{\delta}\ \bar{\rho}\ (1 - \bar{\rho})}{\rho} \tag{5.28}$$

The resulting boundary conditions for Equation 5.28 are:

$$\zeta = \zeta_1 = 0 \quad \text{at } \eta = 0 \tag{5.29}$$

$$\zeta = \zeta_2 = 1/\tilde{\delta} \quad \text{at } \eta = 1 \tag{5.30}$$

In order to obtain a linear second order equation of the form of Equation 5.1, it is necessary to linearize Equation 5.28. The nonlinear term (ζ^2) is therefore quasilinearized in the manner of Lee (Ref. 5.3):

$$(\zeta^2)^{k+1} = (\zeta)^k + 2\ \zeta^k\ (\zeta^{k+1} - \zeta^k) \tag{5.31}$$

where k is the iteration number. Substitution of Equation 5.31 into the non-linear equation (Eq. 5.28) gives the following linear second order, ordinary differential equation:

$$\zeta'' + \left[\frac{2\ Re_s\ \delta^2}{\rho\mu} f^k + \frac{(\rho\mu)'}{\rho\mu}\right]\zeta' - \frac{2\ Re_s\ \delta^3}{\rho\mu}\ \zeta$$

$$= -\ 2\ Res\ \tilde{\delta}\ \left[\bar{\rho}\ \frac{(1 - \bar{\rho})}{\rho\mu} + \frac{\tilde{\delta}^2}{2\ \rho\mu}\ \zeta^{2\,(k)}\right] \qquad (5.32)$$

where the superscript k is used to designate values computed from the previous iteration. Equation 5.32 is now of the form of Equation 5.1 and can therefore be finite-differenced by Equation 5.13 through 5.20 to obtain the following form:

$$A_n\zeta_{n-1} + B_n\zeta_n + C_n\zeta_{n+1} = D_n \qquad (5.33)$$

where

$$A_n = H_n^2 + \alpha_n H_n' \qquad (5.34)$$

$$B_n = G_n^2 + \alpha_n H_n' + \beta_n \qquad (5.35)$$

$$C_n = F_n^2 + \alpha_n F_n' \qquad (5.36)$$

$$D_n = -\ \frac{2\ Res\ \tilde{\delta}}{\rho_n\mu_n}\left[\bar{\rho}\ (1 - \bar{\rho}) + \tilde{\delta}^2\zeta_n^{2\,(k)}\right] \qquad (5.37)$$

$$\alpha_n = \frac{2\ Res\ \tilde{\delta}^2\ f_n{}^k}{(\rho\mu)_n} + \frac{(\rho\mu)_n'}{(\rho\mu)_n} \qquad (5.38)$$

and

$$\beta_n = -\ 2\ Re_s\ \tilde{\delta}^3 \qquad (5.39)$$

Finite-differencing at each station yields the following matrix equation,

$$\begin{bmatrix} B_2 & C_2 & & & & & \\ A_3 & B_3 & C_3 & & & & \\ & A_4 & B_4 & C_4 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & A_{s-1} & B_{s-1} \end{bmatrix} \cdot \begin{bmatrix} \zeta_2 \\ \zeta_3 \\ \\ \cdot \\ \cdot \\ \cdot \\ \zeta_{s-1} \end{bmatrix} = \begin{bmatrix} D_2 - A_2\zeta_1 \\ D_3 \\ \\ \cdot \\ \cdot \\ \cdot \\ D_{s-1} - C_{s-1}\zeta_s \end{bmatrix} \tag{5.40}$$

which can be solved by the previously discussed tridiagonal matrix inversion subroutine (TRID).

The f profile is then determined by integration of Equation 5.27,

$$f = \tilde{\delta} \int_{\eta=0}^{\eta=1} \zeta \, d\eta + f_w \tag{5.41}$$

Using a simple trapezoidal scheme (QUAD).

The transformed stand off distance , $\tilde{\delta}$, is computed from f_s (Equation 5.41 evaluated at $\eta=1$) and Equation 5.23 evaluated at $\eta=1$.

$$\tilde{\delta} = - \frac{(\rho v)_s}{2 f_s} \tag{5.42}$$

This computed value of $\tilde{\delta}$ is then compared to the assumed value and a new value estimated. The calculation is repeated until convergence of $\tilde{\delta}$ is achieved ($\Delta\tilde{\delta} \leq 0.001$). The actual standoff distance is then computed as

$$\delta = \tilde{\delta} \int_0^1 \rho \, d\eta \tag{5.43}$$

Again, using the simple trapezoidal scheme (QUAD). Numerical convergence of the momentum solution was verified in the same manner as the elemental equations. In Figure 5.4 a comparison is given of the results of this method to those obtained by Howe and Vegas (Ref. 5.9). The agreement is seen to be quite good.

Energy Equation: The energy equation (Eq. 5.101) is second order and linear in temperature and therefore does not require quasilinearization. Finite-differencing Equation 3.101 using the difference approximations of Equations 5.13 and 5.14 gives,

$$A_n T_{n-1} + B_n T_n + C_n T_{n+1} = D_n \tag{5.44}$$

where

$$A_n = H_n^2 + \alpha_n H_n^1 \tag{5.45}$$

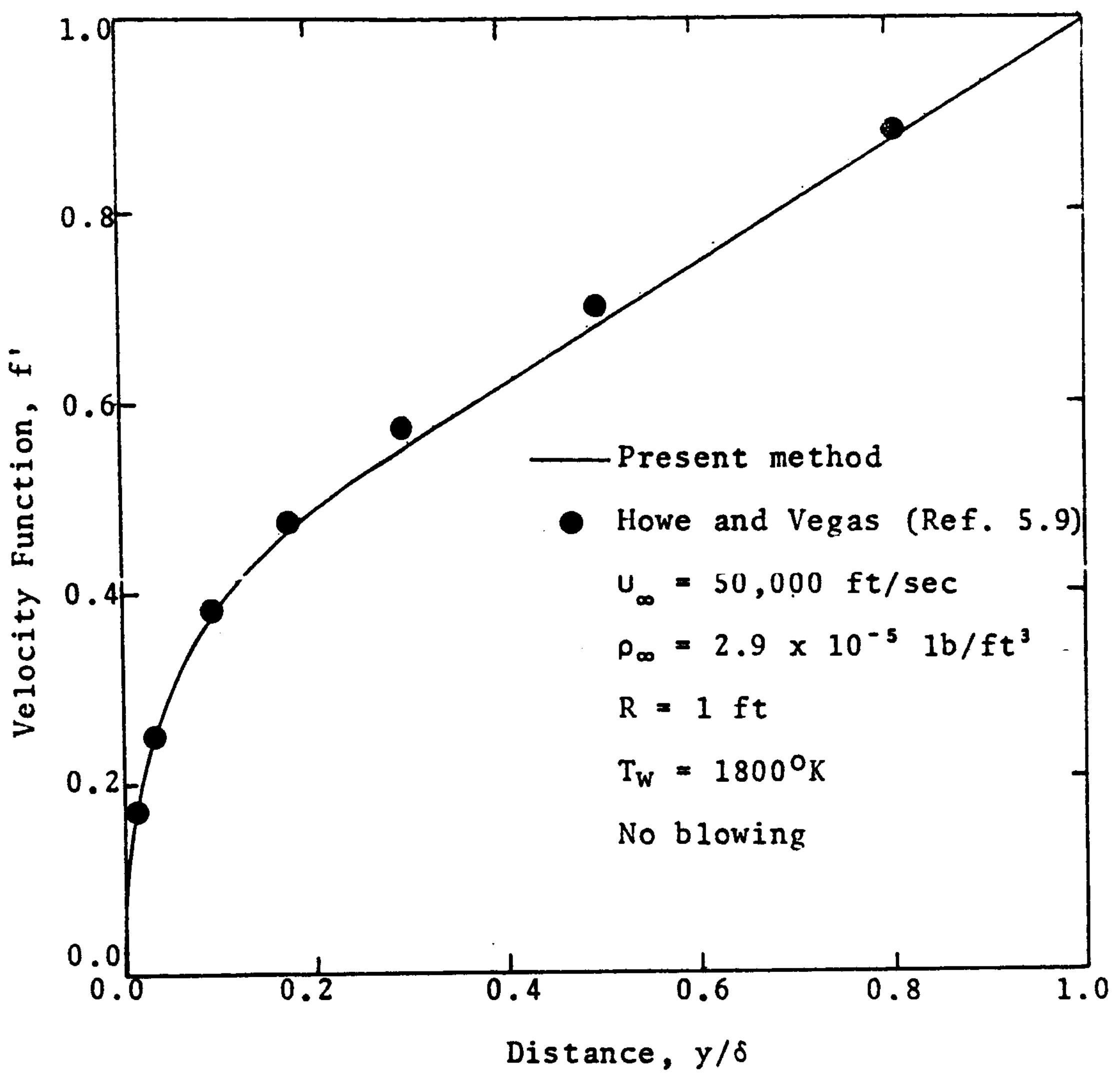

Figure 5.4. Comparison of Stagnation Line Momentum Equation Solutions (Ref. 5.2).

$$B_n = G_n^2 + \alpha_n \; G_n^1 \tag{5.46}$$

$$C_n = F_n^2 + \alpha_n \; F_n^1 \tag{5.47}$$

$$D_n = \frac{\tilde{\delta}}{\rho_n k_n} \left[\rho_n v_n^2 \left(\frac{dv}{dn}\right)_n + \left(\frac{dq_R}{dn}\right)_n \right] \tag{5.48}$$

and

$$\alpha_n = - \frac{\tilde{\delta}}{2\rho_n k_n} \left[\rho_n v_n C_{p_n} - 2 \left(\frac{d(\rho k)}{dn}\right)_n \right] \tag{5.49}$$

In Chapter III, it was noted that the wall boundary condition for the energy equation is simply the equilibrium sublimation temperature (T_W) of the ablator. The sublimation temperature of the phenolic-nylon ablator* employed in this study was 3450°K (±25°K) at one atmosphere pressure. The shock temperature (T_S) was determined from the Rankine-Hugoniot Equations (Eqs. 3.81-3.84).

By applying the finite-differential formulation of the energy equation (Eq. 5.44) at each station across the flowfield, the following matrix equation results,

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$$\begin{bmatrix} B_2 & C_2 & & & & \\ A_3 & B_3 & C_3 & & & \\ & A_4 & B_4 & C_4 & & \\ & & \cdot & \cdot & \cdot & \\ & & & \vdots & \vdots & \ddots \\ & & & & A_{s-1} & B_{s-1} \end{bmatrix} \cdot \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ \vdots \\ T_{s-1} \end{bmatrix} = \begin{bmatrix} D_2 - A_2 T_1 \\ D_3 \\ D_4 \\ \vdots \\ D_{s-1} - C_{s-1} \; T_s \end{bmatrix} \tag{5.50}$$

*The elemental composition of this ablator was C_C = 0.7303, C_H = 0.0729, C_H = 0.0729, C_N = 0.0496, and C_O = 0.1472.

As with the previous solutions of tridiagonal matrices, Equation 5.50 was solved by the algorithm given by Conte (Ref. 5.1) and programmed in the Fortran subprogram, TRID. In the same manner as the elemental and momentum solutions, numerical convergence of the energy equation was demonstrated for $\Delta T/T_s \leq 0.05$ from one grid point to the next.

Overall Analysis

The previously discussed numerical solutions were incorporated with the chemical equilibrium calculations (CHEMEQ),* the properties package (PROPRT), and the radiative heating analysis (LRAD), in a Fortran program designated as SLAB (Stagnation Line Analysis with Binary Diffusion). A simplified flow diagram of this overall analysis was given in Figure 5.1.

Verification of the Overall Analysis: As previously shown, each of the subprograms used in this program were independently tested both for numerical convergence and agreement with other investigators. In order to test the overall analysis, a comparison was made between the dimensionless radiative heating rates predicted by the SLAB program and the predictions of other investigators. For these no mass injection cases

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*Presented and verified in Appendix E.

which are shown in Figure 5.5, the comparison is quite favorable. It should be noted that the results of Rigdon, et al., are based on the most rigorous radiation analysis of those presented and that the predictions of SLAB are in excellent agreement with these results.

Computational Experience with the Overall Analysis: Computer running time presented the major difficulty in the current study. The radiation calculation alone required approximately 2.5 minutes for a sweep of the finite difference grid;* the chemical equilibrium calculation correspondingly required approximately 1.0 minutes. The remaining calculations required a total of approximately 0.5 minutes. A single pass through the outer loop (See Figure 5.1) required one radiation (LRAD) calculation and 12-15 chemical equilibrium calculations (CHEMEQ), thus requiring a total of 15-18 minutes for each major (outer loop) iteration. Depending upon the initial estimates, the overall solution required from 3 to 20 major iterations. In terms of execution time this amounted to about 6.0 hours.**

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*For approximately 59 finite-difference stations.

**It is felt that the execution time could possibly be reduced by as much as one-sixth of that presently required. A discussion of the proposed modifications is included in Chapter VII on Conclusions and Recommendations.

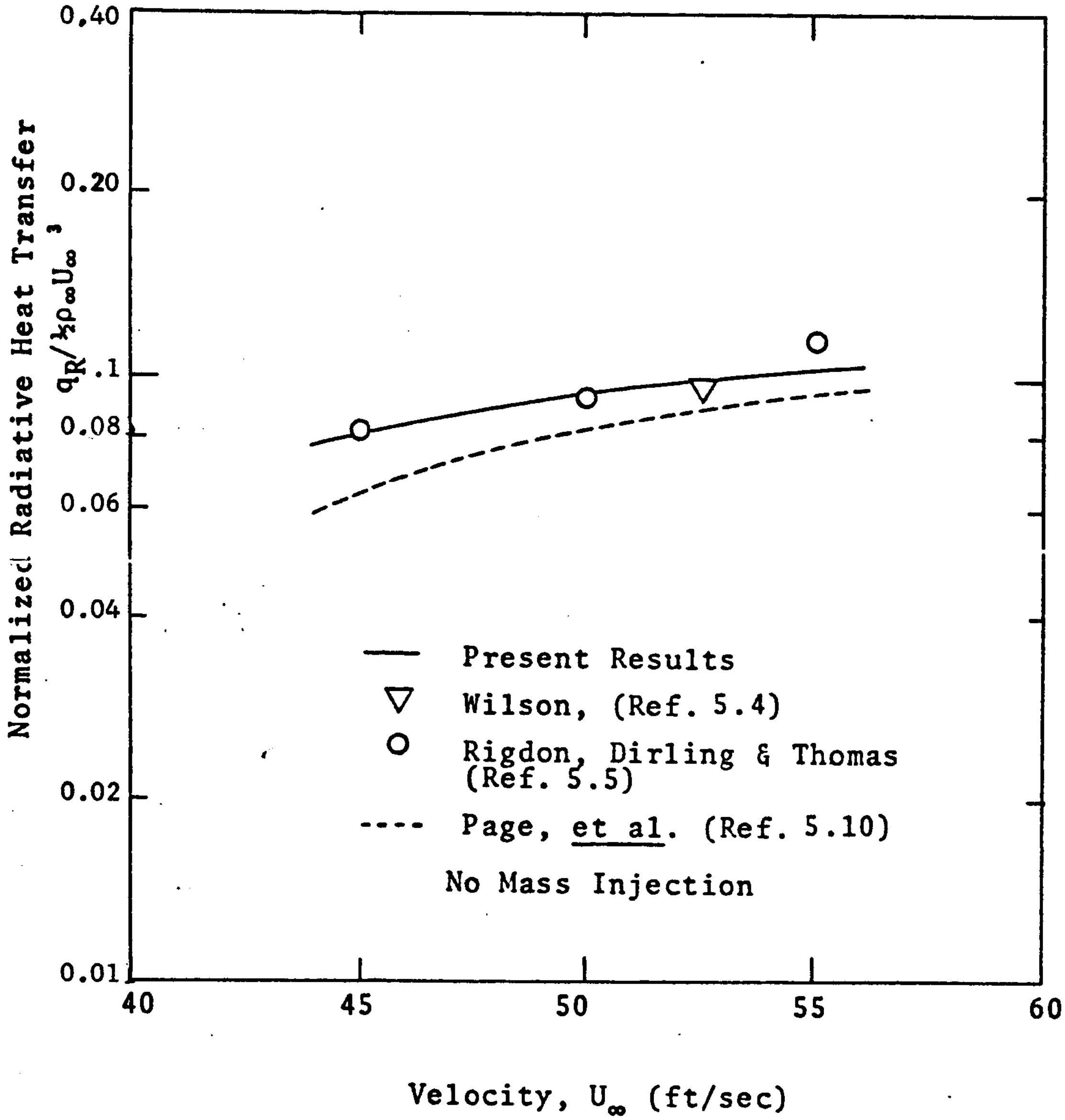

Figure 5.5. Comparison of Dimensionless Radiative Heating Rates (P_s = 1.0 atm, R = 9 ft.).

The above mentioned run times are of course dependent upon the number of steps employed in the numerical analysis. In fact, a direct proportionality was observed. Therefore, it is desirable to minimize the number of steps considered. In the current study it was found that the converged solutions could be obtained with 55-59 steps using an optimum, variable-stepsize distribution. It is felt that this number of steps represents the minimum possible for the flight conditions investigated.

Another source of difficulty encountered in this study is the extreme sensitivity and nonlinearity of the radiative flux divergence. The extent of this problem is illustrated in Figure 5.6, which demonstrates the pervasive effect of a small, localized variation in the temperature distribution upon the flux divergence profile. The sharp ridge appearing in the flux divergence at the stagnation point was typical of the cases studied.* Furthermore, the irregular behavior of the flux divergence in the region of the stagnation point did not cease until the temperature profile was nearly converged. Because of these adversities in the radiative flux divergence, it was very tedious to

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*It should be pointed out that this phenomena is also observed in the results of Wilson (Ref. 5.4) and Rigdon, et al. (Ref. 5.5).

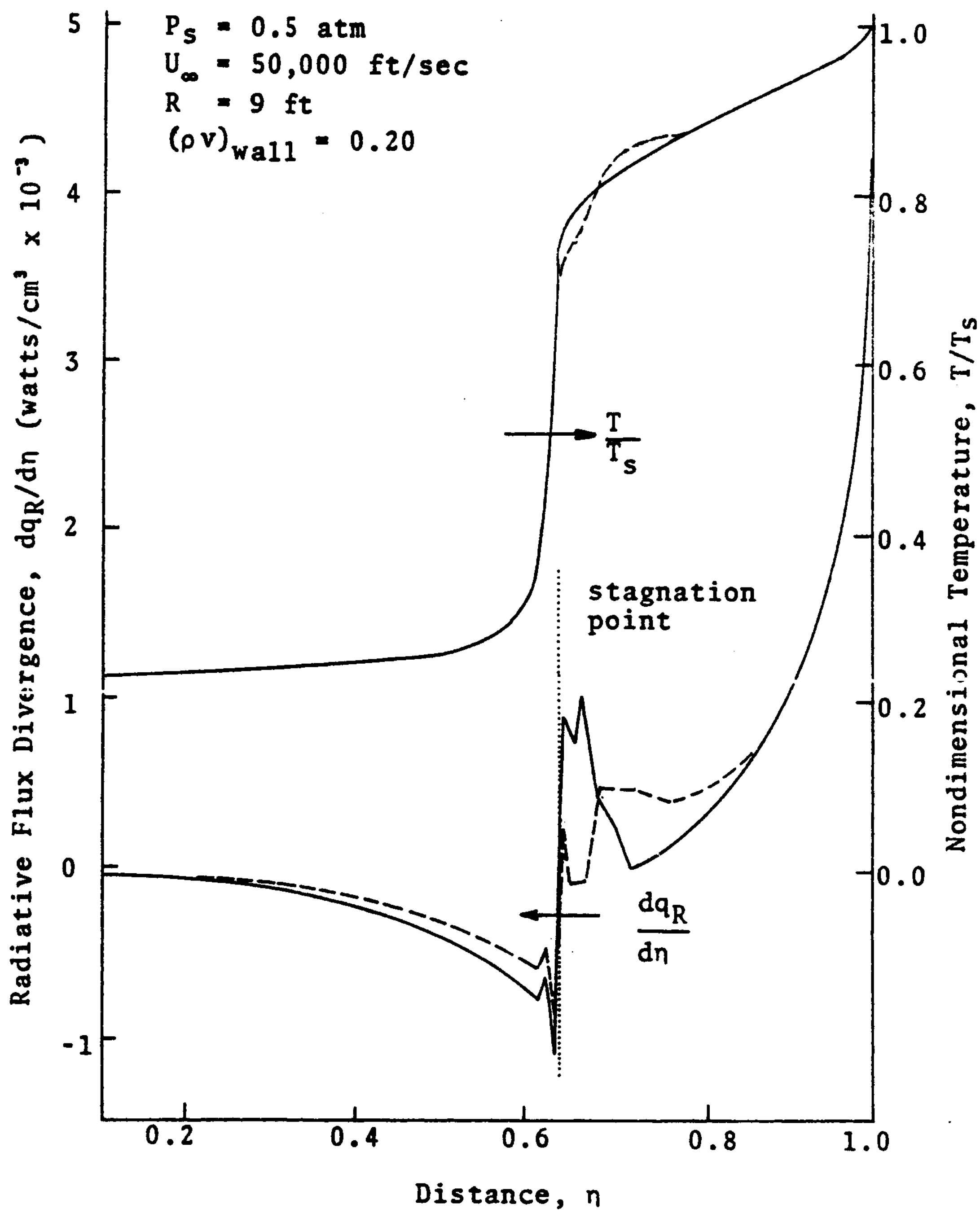

Figure 5.6. Illustration of the Effect of Temperature Variations Upon Radiative Flux Divergence.

achieve convergence. The best results were obtained by weighting the estimated temperature profiles by means of the following relationship

$$T_{new} = 0.65\ T_{calc} + 0.35\ T_{old} \qquad (5.51)$$

where T_{calc} is the computed temperature distribution based upon a flux divergence profile computed from T_{old}. On occasion it was observed that if T_{new} differed significantly (>10%) from T_{old}, a divergence would occur in the numerical solution from which it could not recover. Therefore, a maximum of 8% variation was permitted in the temperature change from iteration to iteration.

The initial estimates for each case were obtained from the analysis by Engel (VISRAD III, Ref. 5.6). The analysis includes mass injection of ablation products with radiation coupling, but assumes air properties throughout the shock layer and a step-function representation of the elemental distribution. For low blowing cases, VISRAD was found to agree quite well with the SLAB analysis. However, for large blowing some differences were noted in the temperature profile.

The typical progress of the SLAB analysis from iteration to iteration is given in Figure 5.7 to 5.11. As the solution was approached (Fig. 5.8) instability

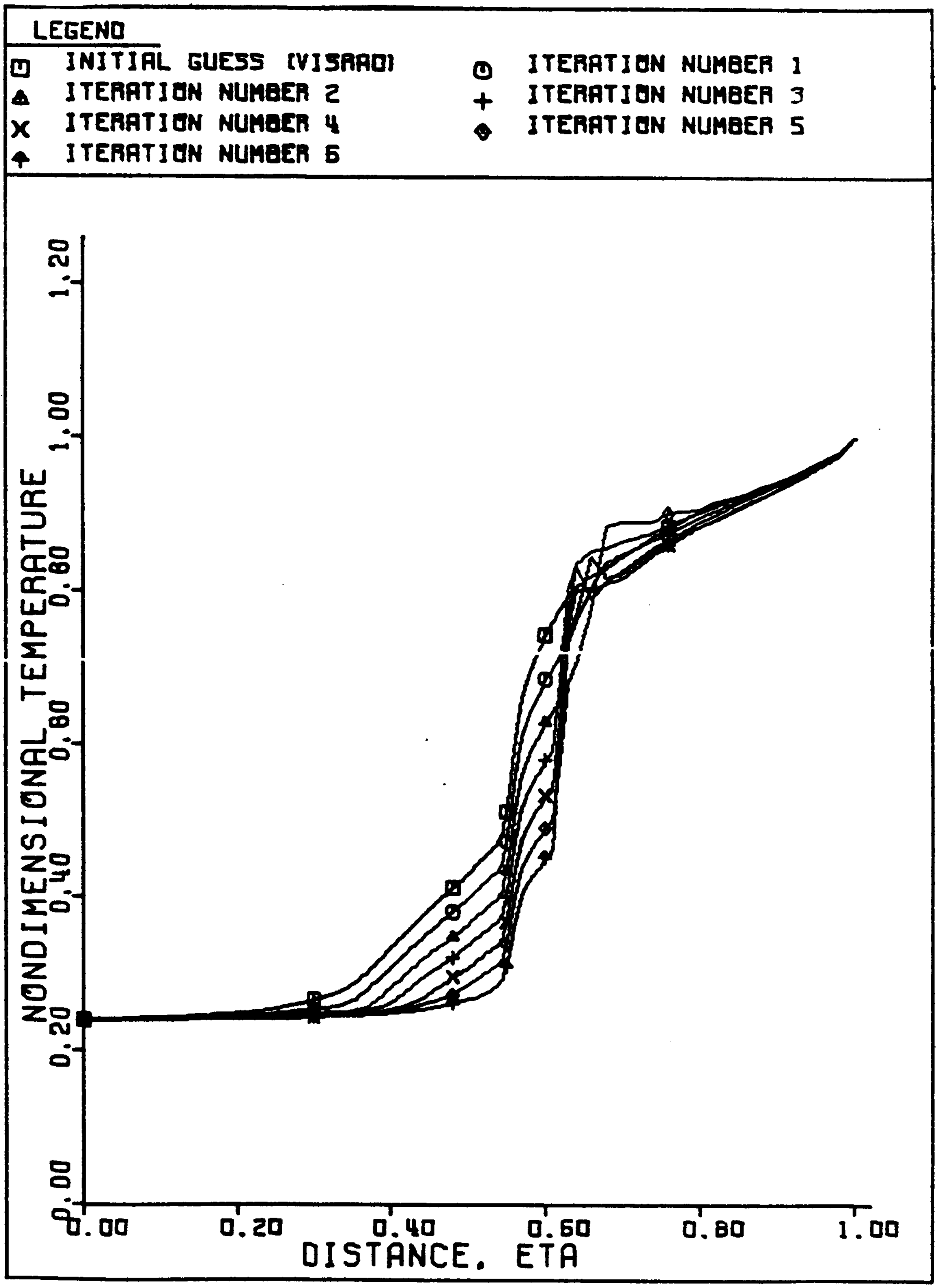

Figure 5.7. Variation in Temperature Profiles From Iteration to Iteration.

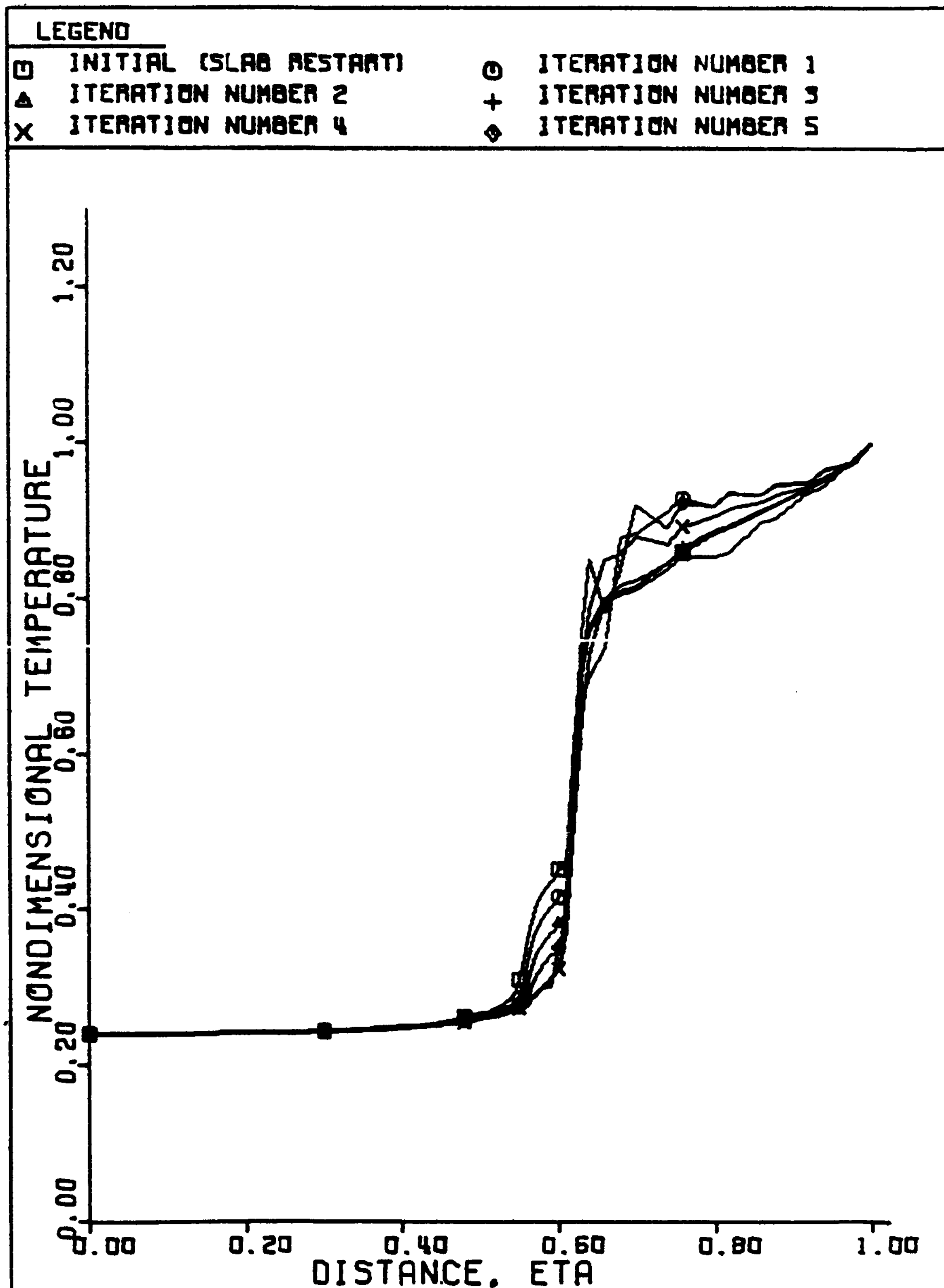

Figure 5.8. Variation in Temperature Profiles From Iteration to Iteration.

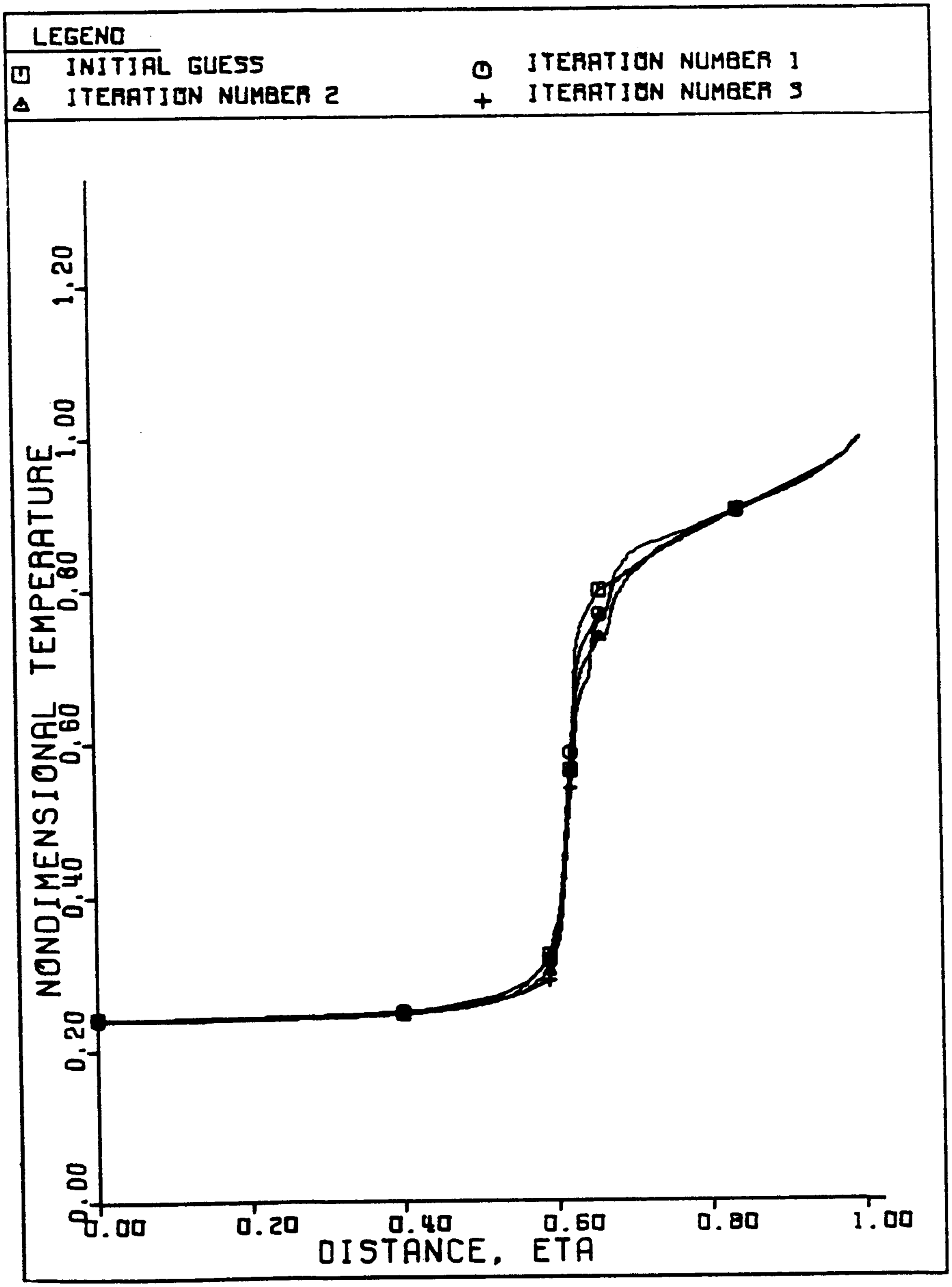

Figure 5.9. Variation in Temperature Profiles From Interation to Iteration.

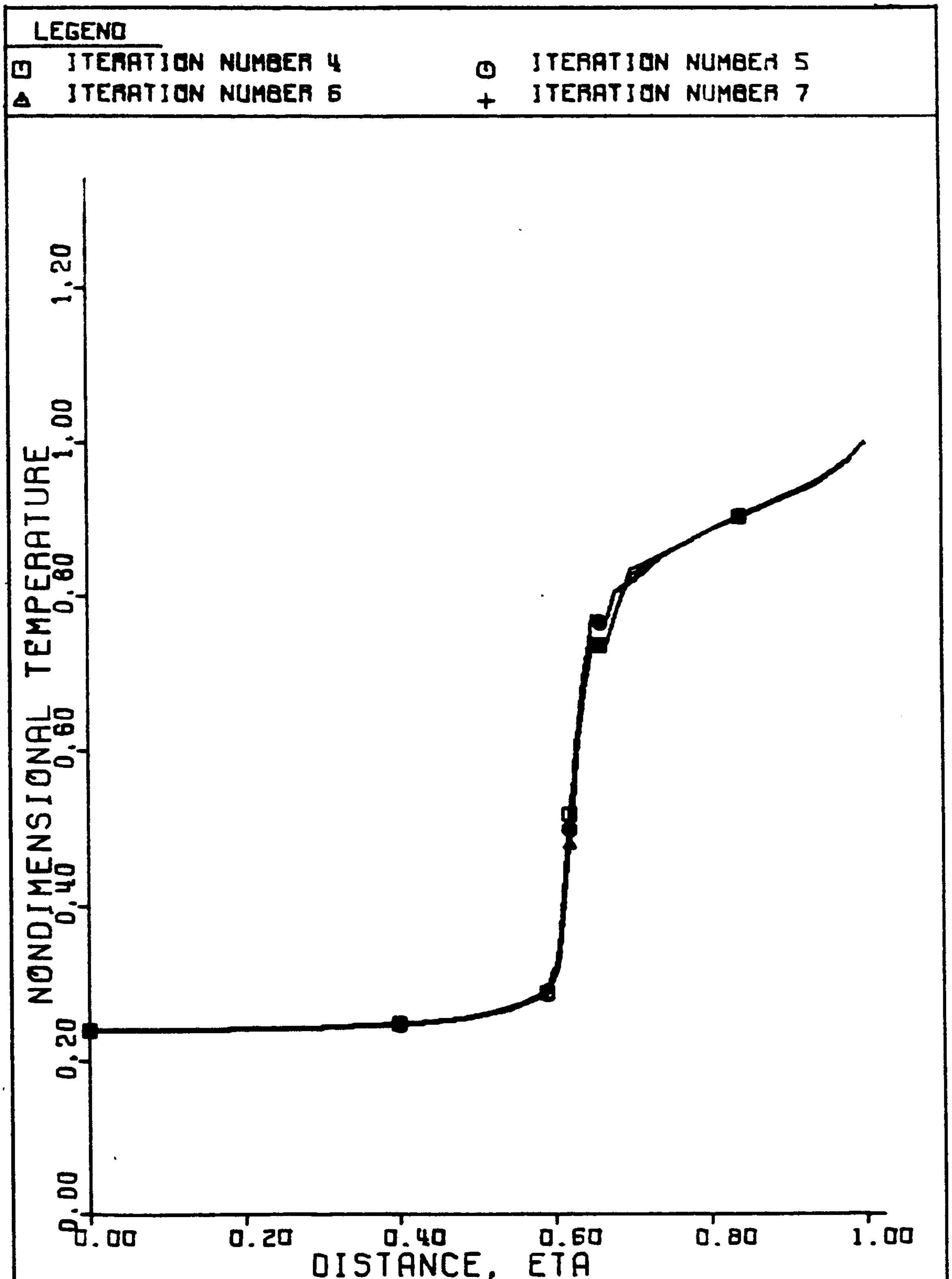

Figure 5.10. Variation in Temperature Profiles From Iteration to Iteration.

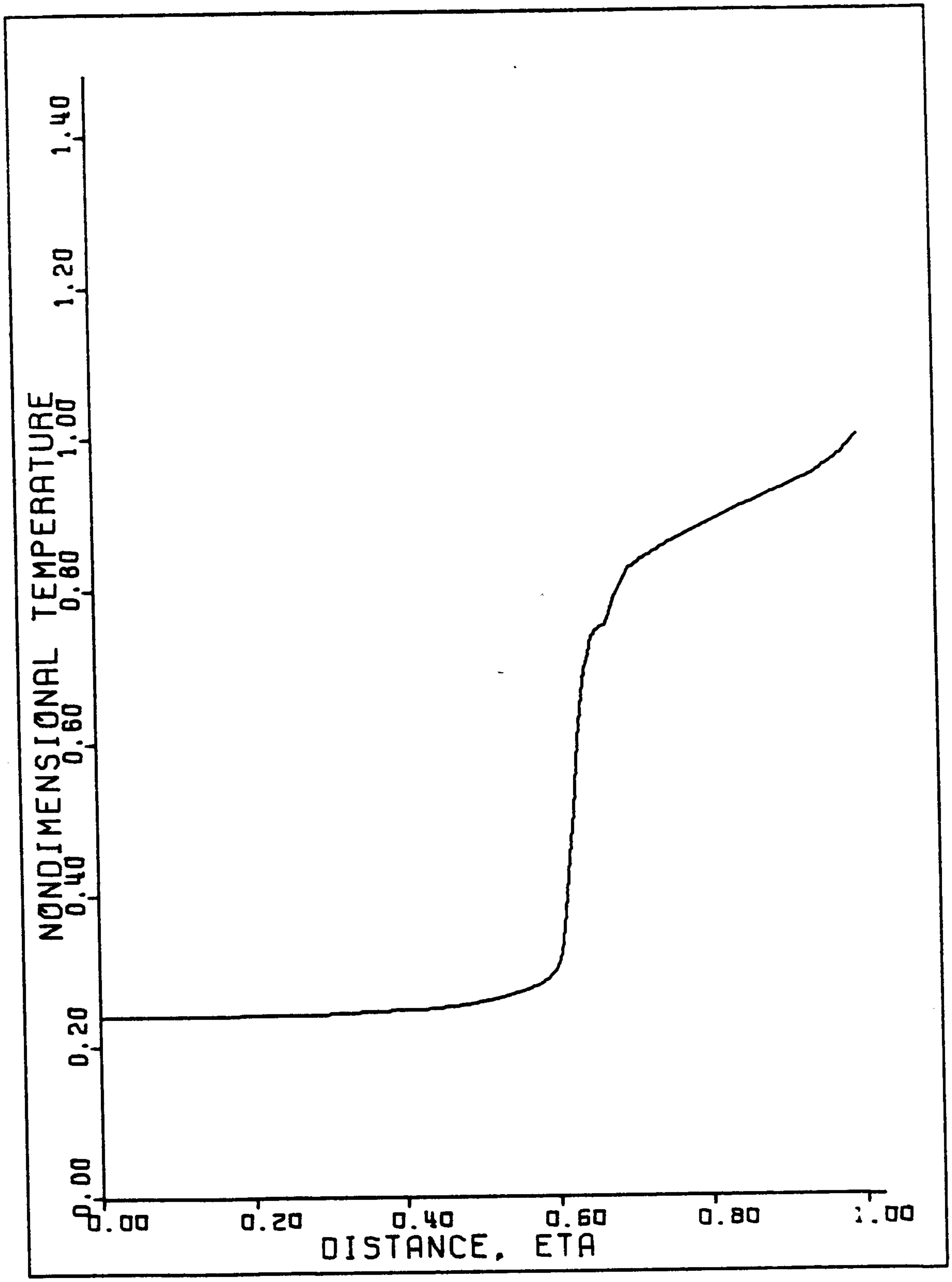

Figure 5.11. Converged Temperature Profile.

began to occur in the higher temperature region. Therefore, the stepsize distribution was revised to conform to the new profile. The program was then restarted from the third iteration of Figure 5.8. The resulting progress to convergence is seen in Figures 5.9, 5.10, and 5.11.

Stagnation Region Heating Analysis with Multicomponent Diffusion

Because of the extensive time requirements of the overall stagnation line analysis (~6.0 hours) fully coupled multicomponent diffusion calculations were not performed. Instead, a partial coupling was obtained by using the temperature and velocity profiles computed from the corresponding binary (SLAB) analysis. The resulting species distributions were then used with the given temperature profile in a radiative heating analysis (LRAD). The resulting values of wall heating rates and radiative flux divergence profiles were then compared with those obtained from the corresponding SLAB analysis. The details of the multicomponent diffusion analysis (SLAM) are given in the following discussion.

Species Solution with Multicomponent Diffusion: Because the Stefan-Maxwell Equations (Eqs. 3.98) are implicit in the mass flux (J_i), there exists no direct method by which a simultaneous solution with the elemental continuity equations (Eqs. 3.97) can be obtained. Without further simplification of the Stefan-Maxwell equations (e.g., the bifurication approximation), it is therefore necessary to resort to an iterative numerical method such as that developed in the current study. In the following development it is shown that the elemental mass fluxes ($\tilde{J}_j$) can be rigorously expressed in terms of an effective elemental diffusion coefficient ($\tilde{D}_j$).

Effective Elemental Diffusion Coefficients: It was shown in Chapter II that a rigorous multicomponent expression for the species mass fluxes (J_i), could be written as follows:

$$J_i = - \rho D_i \frac{dC_i}{dy} \tag{5.52}$$

where D_i is an effective species diffusion coefficient which can be computed from Equation 2.22. A Shvab-Zeldovitch transformation of Equation 5.52 yields

$$\tilde{J}_j = - \rho \tilde{M}_j \sum_i \frac{A_{ij} D_i}{M_i} \frac{dC_i}{dy} \tag{5.53}$$

By defining:

$$\tilde{D}_j = \frac{\tilde{M}_j \sum \frac{A_{ij} D_i}{M_i} \frac{dC_i}{dy}}{\frac{d\tilde{C}_j}{dy}} = \text{effective elemental diffusion coefficient of element "j"} \qquad (5.54)$$

Equation 5.53 can be written as:

$$\tilde{J}_j = -\rho \tilde{D}_j \frac{d\tilde{C}_j}{dy} \qquad (5.55)$$

Upon performing a Dorodnitzn transformation (Eq. 3.93), Equation 5.55 can be substituted into the transformed elemental continuity equations (Eqs. 3.97) to give the following results,

$$\frac{d^2 C_j}{d\eta^2} + a_1 \frac{dC_j}{d\eta} = 0 \qquad j = 1, 2, \ldots, \ell \qquad (5.56)$$

where

$$a_1 = 2 \frac{d \ln \rho}{d\eta} + \frac{d \ln \tilde{D}_j}{d\eta} - \frac{v\tilde{\delta}}{\rho \tilde{D}_j} \qquad (5.57)$$

With the exception of the diffusion coefficients, the previous equations are identical to the binary elemental formulations (Eqs. 5.3 and 5.4). As with the binary formulations, the following wall boundary conditions exist:

$$\rho v \tilde{C}_j - \frac{\rho^2 \tilde{D}_j}{\tilde{\delta}} \frac{d\tilde{C}}{d\eta} = \tilde{I}_j \qquad (5.58)$$

The shock boundary conditions were again expressed as the equilibrium composition of air at the shock temperature (T_s).

Assuming effective elemental diffusion coefficient profiles, the corresponding elemental distributions can be determined in the same manner as with the previously discussed binary diffusion analysis. From the elemental distributions and the temperature profiles the equilibrium species compositions can be determined.

From the Stefan-Maxwell Equations (Eqs. 3.98):

$$\frac{\rho}{\tilde{\delta}} \frac{dY_i}{d\eta} = \sum_{\substack{j=1 \\ j \neq i}}^{\nu} \frac{Y_i Y_j}{ij} (V_j - V_i) \quad i=1, 2, \ldots, \nu-1 \quad (3.98)$$

and the sum of the mass fluxes based upon the assumption of a mass averaged velocity (Eq. 2.13, $\sum \rho_i V_i = 0$), the diffusion velocities corresponding to the estimated species distribution can be determined. A solution of the following matrix is thus required at each finite-difference station in the flowfield.

$$\begin{bmatrix} -\sum\limits_{j\neq 1}\frac{Y_j}{\mathcal{D}_{1j}} & \frac{Y_2}{\mathcal{D}_{12}} & \cdots & \frac{Y_{\nu-1}}{\mathcal{D}_{1,\nu-1}} & \frac{Y_\nu}{\mathcal{D}_{1\nu}} \\ \frac{Y_1}{\mathcal{D}_{21}} & -\sum\limits_{j\neq 2}\frac{Y_j}{\mathcal{D}_{2j}} & \cdots & \frac{Y_{\nu-1}}{\mathcal{D}_{2,\nu-1}} & \frac{Y_2}{\mathcal{D}_{2\nu}} \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \frac{Y_1}{\mathcal{D}_{\nu-1}} & \frac{Y_2}{\mathcal{D}_{\nu-1,2}} & \cdots & -\sum\frac{Y_j}{\mathcal{D}_{\nu-1,j}} & \frac{Y_\nu}{\mathcal{D}_{\nu-1,\nu}} \\ \rho_1 & \rho_2 & \cdots & \rho_{\nu-1} & \rho_\nu \end{bmatrix} \cdot \begin{bmatrix} V_1 \\ V_2 \\ \cdot \\ \cdot \\ \cdot \\ V_{\nu-1} \\ V_\nu \end{bmatrix} = \begin{bmatrix} \frac{\rho}{\delta Y_1}\frac{dY_1}{d\eta} \\ \frac{\rho}{\delta Y_2}\frac{dY_2}{d\eta} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\rho}{\delta Y_{\nu-1}}\frac{Y_{\nu-1}}{d\eta} \\ 0 \end{bmatrix} \tag{5.59}$$

The solution to this set of equations was implemented in the Fortran Subprogram, MCD, a listing of which appears in Appendix C. The analysis employed in MCD was verified by a comparison with results obtained from an analytical solution reported by Toor (Ref. 5.7).* This comparison is given in Figure 5.12 and reveals excellent agreement between the numerical and analytical predictions. The figure also demonstrates the capability of the current analysis to predict the cross-effects discussed with reference to Figure 2.1 from which the analytical values were taken.

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*Also given in Figure 2.1.

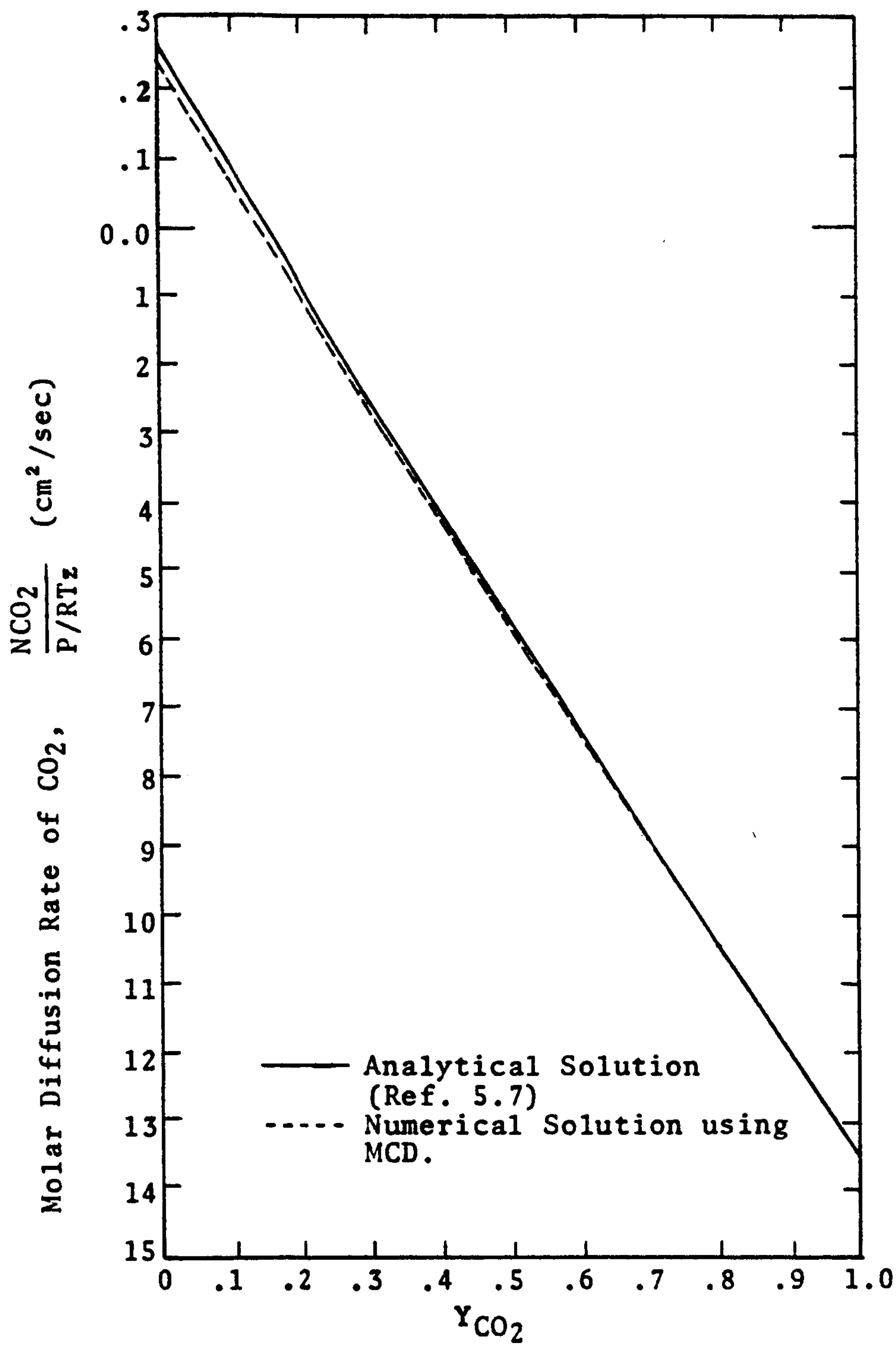

Figure 5.12. Diffusion Rates of CO_2 As a Function of Y_{CO_2} (Ref. 5.7).

The species mass fluxes are determined in MCD from the following relationship,

$$J_i = \rho_i V_i \tag{5.60}$$

Using the Shvab-Zeldovitch transformation (Eq. 3.21), the elemental mass fluxes are then computed in the subprogram EFLUX:

$$\tilde{J}_j = M_j \sum_{i=1}^{\nu} \frac{A_{ij} J_i}{M_i} \tag{3.21}$$

An estimate of the effective elemental diffusion coefficients is then obtained from the Dorodnitzn transform of Equation 5.55:

$$\tilde{D}_{j\,calc} = - \frac{\tilde{\delta}\ \tilde{J}_j}{\rho^2 \dfrac{dC_j}{d\eta}} \tag{5.61}$$

The elemental continuity equations (Eqs. 5.56) are again solved using a revised estimate of the diffusion coefficients from the following relationship (DIJ):

$$\tilde{D}_j(\eta)_{new} = 0.7\left(- \frac{\tilde{\delta}\ \tilde{J}_j(\eta)}{\rho^2 \dfrac{d\tilde{C}_j(\eta)}{d\eta}}\right) + 0.3\ \tilde{D}_j(\eta)_{old} \tag{5.62}$$

This iterative procedure is thus repeated until all of the elemental mass fractions from one iteration to the next agree within 1%. The density profile is then updated and above process repeated. When the density profile has converged to 5%, the overall multicomponent diffusion analysis is said to be converged. A simplified flow-diagram of the previously described iterative procedure is given in Figure 5.13.

Electron Diffusion: In the current study, the ambipolar diffusion has been assumed to describe the diffusion behavior of the electron. This assumption implies that the electron diffuses at the same rate as the parent dissociated atom, or that throughout the flowfield the density of electrons (ρ_{e^-}) is equal to the total density of the ionized atoms (e.g., O^+, N^+, and C^+):

$$\rho_{e^-} = \rho_{c} + \rho_{n^+} + \rho_{o^+} \tag{5.63}$$

For the purpose of the chemical equilibrium calculation (see Appendix E), the electron has been treated as an elemental component of the undissociated molecules.* For example, N is said to be composed of two "elements": N^+ and e^-. The basic "elements" are then C^+, H, O^+, N^+ and e^- (neglecting hydrogen ionization). Assuming ambipolar diffusion, the elemental composition of electrons at any point in the flowfield

*The assumption is a standard procedure in dealing with equilibrium studies of dissociated gases (Refs. 5.4 and 5.5).

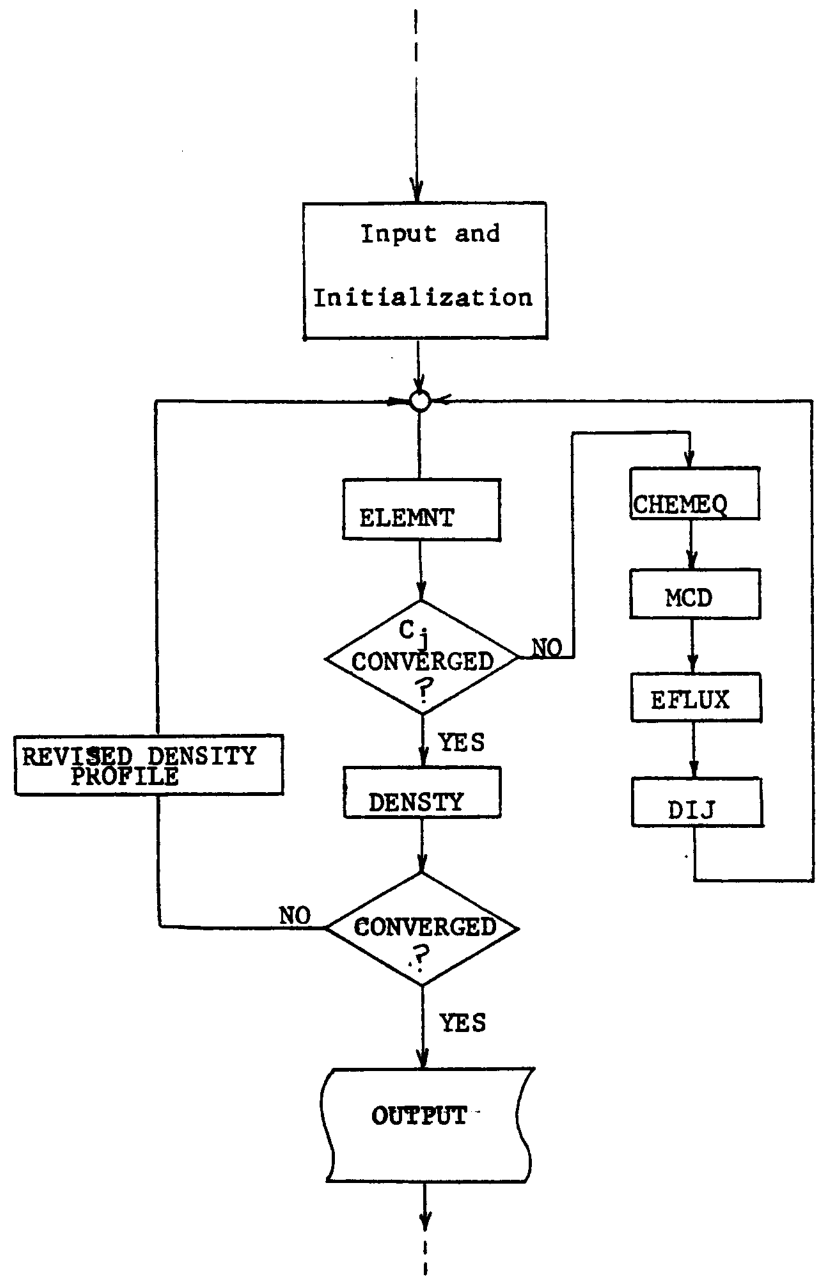

Figure 5.13. Simplified Flow Diagram of Species Solution with Multicomponent Diffusion.

is therefore related to the elemental compositions of C^+, O^+, and N^+ by the following equation:

$$\tilde{C}_{e^-} = \left[\frac{\tilde{C}_{c^+}}{\tilde{M}_{c^+}} + \frac{\tilde{C}_{o^+}}{\tilde{M}_{o^+}} + \frac{\tilde{C}_{n^+}}{\tilde{M}_{n^+}} \right] \tilde{M}_{e^-} \qquad (5.64)$$

Numerical Difficulties: It has been noted that as the elemental diffusion effects become small (i.e., as $|\tilde{J}_j|$ becomes much less than ρv), the use of Equation 5.61 leads to eratic predictions of the elemental diffusion coefficients ($\tilde{D}_j$). These irregularities, occuring in the convection dominated regions, are frequently sufficient in magnitude to prevent convergence of the overall solution. This problem is partially overcome by setting the elemental diffusion coefficients equal to a small number (10^{-6}) for all values outside of the diffusion zone. The diffusion zones of each element are specified as the regions in which

$$\tilde{J}_j/\rho v \geq 0.01 \qquad j=1, 2,\ldots,\ell \qquad (5.65)$$

The establishment of this diffusion region results in discontinuities in the diffusion coefficient profiles at the extremities of the zone. These discontinuities are amplified by the derivative term ($d\ln\tilde{D}_j/d\eta$) appearing in the elemental continuity equations

(Eqs. 5.56 and 5.57) and quite often make convergence difficult to achieve. Since the predicted coefficients have been observed to be relatively constant across the diffusion zone, it was felt that the derivative term ($d\ln D_j/d\eta$) could be neglected without significant losses in accuracy. In Figure 5.14, a comparison is given between typical elemental profiles computed with and without the $d\ln D_j/d\eta$ term, and with the corresponding binary diffusion profile. From these results, the error in heating rate arising from the omission of the derivative term was found to be negligible in comparison to the corresponding binary diffusion results.

<u>Summary</u>

The details of the numerical implementation of each of the conservation equations have been given. The resulting Fortran subprograms have been individually tested and found to be functioning properly. These numerical solutions have been combined with the transport, thermodynamic, and radiation property models, discussed and verified in previous chapters, in a Fortran computer program (SLAB) which has been shown to yield heating rate predictions which are in excellent agreement with similar existing analyses. In addition, an implicit multi-component diffusion analysis (SLAM) has been developed and verified by comparison with analytical results.

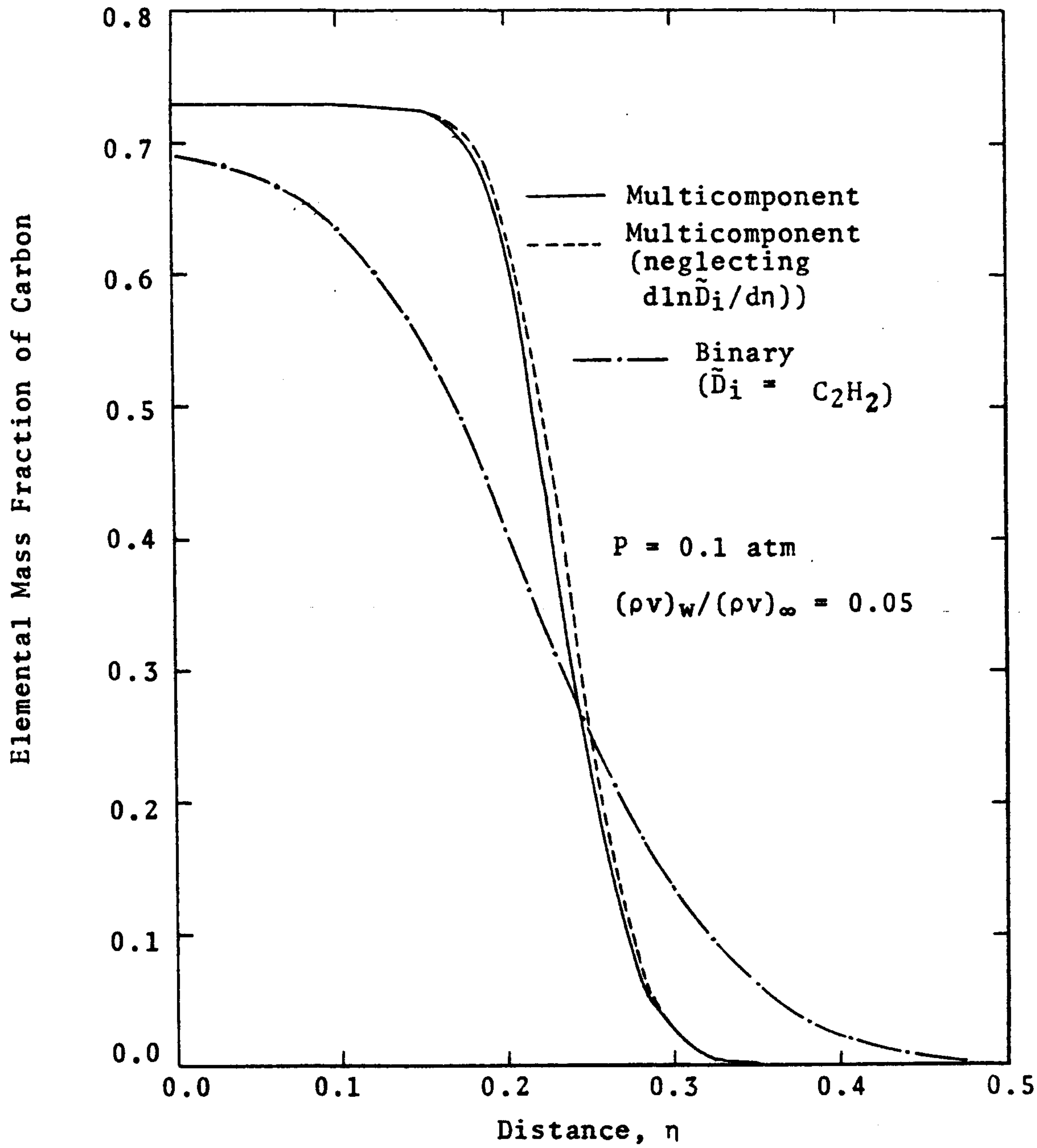

Figure 5.14. Comparisons of Numerical Results With and Without $d\ln\tilde{D}_i/d\eta$.

These analyses provide the necessary tools for an accurate assessment of the transport phenomena occurring in the multicomponent, reacting flowfields surrounding and interacting with ablative thermal protection systems. In the following chapter, the results of the current study of a phenolic-nylon ablator, exposed to a high velocity entry condition, are presented.

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CHAPTER VI

RESULTS OF STAGNATION REGION HEATING ANALYSES

Typical trajectories for earth·entry from space origins are shown in Figure 6.1. As discussed in Chapter I, the increase in entry velocities over lunar return missions is such that radiation heating becomes the governing factor in the design of thermal protection systems. Because of the tremendous success and the corresponding advanced state of technology associated with charring ablators of the Apollo shape, it is indeed desirable to fully explore the possibilities of employing the same type of heat protection system for return missions from planetary flight.

Several studies have been made of the effectiveness of charring ablators in blocking the radiation heat transfer during high velocity re-entry (Refs. 6.1-6.4). It has been shown from these studies that ablation product absorption is effective in reducing the radiation heat flux to the vehicle surface. However, in an effort to simplify the required calculations these

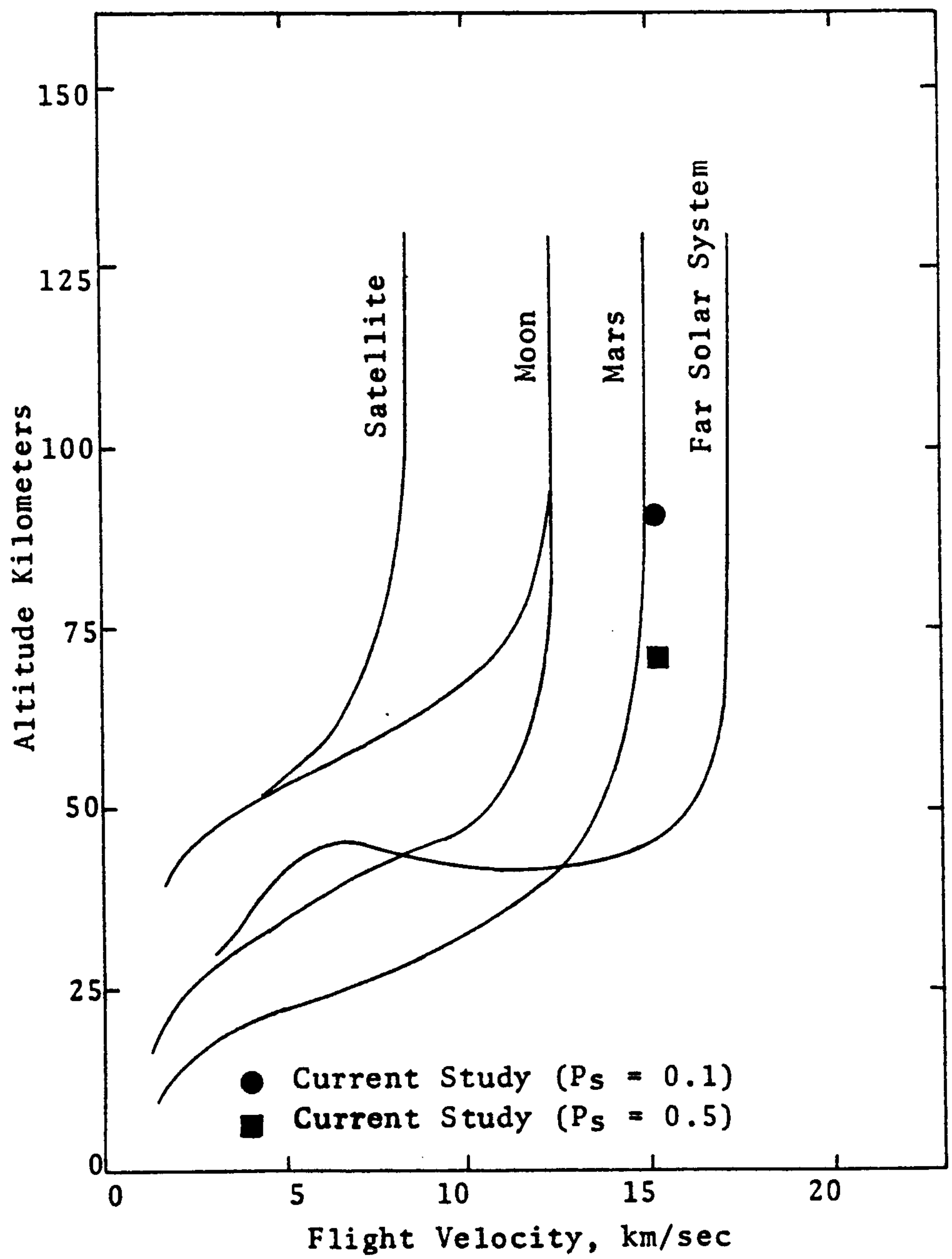

Figure 6.1. Typical Trajectories for Earth Entry From Space Origins (Ref. 6.5).

investigators have all neglected the effects of multi-component diffusion. In most cases, air transport and thermodynamic properties have also been assumed for the injected ablation products. Furthermore, with the exception of a single case for a pure graphite ablator (Ref. 6.2), the previously mentioned studies have concentrated on a specific carbon-phenolic ablator.

The reasoning for the selection of ablators with high carbon content is based upon the fact that atomic carbon is an excellent absorber of radiant energy. However, as observed by Rigdon (Ref. 6.2), the pure graphite ablator was found to be <u>less effective</u> in reducing radiant heating effects than the carbon-phenolic blend. Two observations can be made from this result. First, the increase in heating (relative to the carbon-phenolic ablator) is most likely attributable to re-radiation by the atomic carbon which occurs as the temperature is increased by the absorption process. Secondly, this analysis by Rigdon includes <u>air</u> thermodynamic and transport properties for the ablation products. The use of the correct properties could significantly affect the results of this analysis.

The foregoing discussion leads directly to the objectives of the current study. First of all, what are the effects on heating rate predictions of assuming a computationally more simple binary diffusion model (or no diffusion as in Ref. 6.3) as opposed to a rigorous multicomponent diffusion analysis? Secondly, what are the effects of assuming simplified (air) transport and thermodynamic properties for the injected ablation products? Finally, how do other ablators compare to carbon-phenolic and graphite in reducing radiation heating of high-velocity entry vehicles? The indications are that an optimum blend of ablation products exists.

In this study, a rigorous computer analysis (SLAB)* was developed to accurately determine the effectiveness of given ablative materials in reducing radiation heating of entry vehicles. The analysis, which has been described and verified in the previous chapters, includes a capability for assessing the effects of multicomponent diffusion. In addition, property models have been included to describe the actual

*Listing and input description are presented in Appendix F.

transport and thermodynamic properties for the ablation product and air mixtures encountered in these investigations. This computer analysis, thus provides the necessary tool for answering the above questions relating to the design of ablative thermal protection systems.

The results presented in this chapter are based upon a 40% nylon-60% phenolic resin ablator. The elemental composition of this ablator is compared to that of the previously studied carbon-phenolic ablator in Table 6.1. A body radius of 9.0 feet and an entry velocity of 50,000 feet per second (15.24 km/sec) have also been selected for the current study. In addition two altitudes have been chosen which yield shock layer pressures (P_s) of 0.1 and 0.5 atmospheres.* At an entry velocity of 50,000 ft/sec, a shock pressure of 0.1 atmosphere represents an approximate point in the trajectory where radiation coupling first begins to occur. Shock calculations for this trajectory have shown that the maximum heating occurs near a shock pressure of 0.5 atmospheres. These flight conditions are compared in Figure 6.1 to typical trajectories for earth entry from space origins.

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*Determined from Rankine Hugonoit Equations (Eqs. 3.73-3.76) and selected values of free stream velocity (U_∞) and free stream density (ρ_∞ corresponding to altitude).

TABLE 6.1

COMPARISON OF ELEMENTAL COMPOSITION (MASS PERCENT) OF PHENOLIC-NYLON AND CARBON-PHENOLIC ABLATORS

Element	Phenolic-Nylon	Carbon-Phenolic
C	73.03	92.07
H	7.29	2.16
N	4.96	0.86
O	14.72	4.91
Total	100.00	100.00

A summary of the major flowfield parameters and wall heating results for all cases considered is given in Table 6.2.** As shown in Table 6.2, results have been obtained for the above flight conditions with several variations in transport and thermodynamic properties and in diffusion models. Following a presentation of the ablator-coupled reference cases (i.e., those computed with multicomponent diffusion and exact transport and thermodynamic properties and which are coupled to the ablator response), the effects of these variations will be assessed.

Coupled Ablator-Flowfield Analyses

In order to perform flowfield analyses which are coupled with ablator performance, it is necessary to employ a trial and error solution of the flowfield behavior and the ablator response.* The solution can be accomplished by varying mass injection rates until convergence of wall heating rates is achieved. Due to the excessive computer time requirements (minimum of six hours per case), this procedure was not employed using the SLAB analysis. Instead, parametric studies performed by Engel (Ref. 6.6) with a simplified analysis

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*A discussion of ablator response was presented in Chapter III.

**Graphical results corresponding to each of these cases are given in Appendix H.

TABLE 6.2

SUMMARY OF MAJOR FLOWFIELD PARAMETERS AND CORRESPONDING HEATING RATE PREDICTIONS

Case Number	ρ_∞ (lb/ft)	U_∞ (ft/sec)	$(\rho v)_w$	T_s (^oK)	P_s (atm)	Diffusion Model	Injectant Properties c_p	μ	k	δ (cm)	Wall Heating Rates (watts/cm^2)** q_c	q_R
1*	3.57×10^{-5}	45,000	0.0	14,011	1.0	Binary	--	--	--	10.57	179	5981
2*	2.89×10^{-5}	50,000	0.0	15,044	1.0	Binary	--	--	--	9.48	213	7916
3*	2.41×10^{-5}	55,000	0.0	16,231	1.0	Binary	--	--	--	8.57	255	9588
4	2.85×10^{-6}	50,000	0.05	12,998	0.1	MCD	PN	PN	PN	10.85	120	340
5	2.85×10^{-6}	50,000	0.05	12,998	0.1	Binary	PN	PN	PN	10.85	120	397
6	1.45×10^{-5}	50,000	0.20	14,382	0.5	MCD	PN	PN	PN	13.93	0.3	2022
7	1.45×10^{-5}	50,000	0.20	14,382	0.5	Binary	PN	PN	PN	13.93	0.3	2064
8	2.85×10^{-6}	50,000	0.05	12,998	0.1	Binary	Air	PN	Air	11.38	44	372
9	1.45×10^{-5}	50,000	0.20	14,382	0.5	Binary	PN	PN	Air	13.90	1.2	2104
10	1.45×10^{-5}	50,000	0.20	14,382	0.5	Binary	Air	PN	Air	15.95	0.5	1964

*Cases run to verify overall analysis. These results are presented in Figure 5.4.

**Excluding surface re-radiation.

(VISRAD) were used to obtain an estimate of the ablator-coupled solutions. The VISRAD analysis predicted mass injection rates $[(\rho v)_w/(\rho v)_\infty]$, for the coupled solutions of approximately 0.05 and 0.20 respectively for pressures (P_S) of 0.1 and 0.5 atmospheres. These values were then input to the SLAB program and more accurate heating rates determined. It should be noted that the net radiant heat flux to the ablator surface must include re-radiation from the char (q_{RR}). For these results q_{RR} was determined from the Stefan-Boltzmann Equation:*

$$q_{RR} = \varepsilon\sigma T^4 \tag{6.1}$$

where

$\sigma = 5.6697 \times 10^{-8}$ watts/m^2 $^\circ$K^4

$\varepsilon = 0.66$ (Ref. 6.8)

The total heating of the ablator surface is then,*

$$q_T = q_C + q_R - q_{RR} \tag{6.2}$$

*It is recognized that an approximation has been introduced by handling the re-radiation effect in the above manner. A rigorous approach would require that the appropriate part of the radiation contribution from the ablator surface be included throughout the flowfield in the calculation of the radiation flux divergence. However almost all of the energy re-radiated by the surface occurs below the frequency range of the flowfield. Consequently, the gas is optically thin with respect to this radiation, and this energy is not absorbed. An assessment of the effect of the small amount of energy in the frequency range that is absorbed is given by Engel (Ref. 6.6) which shows that this effect is of no consequence.

The total wall heating rates and the corresponding mass injection rates for the 0.1 and 0.5 atmosphere cases were then compared to the ablator response curves. These results are shown in Figure 6.2 and clearly show that the ablator-coupled solution is well approximated by the assumed mass injection rates. In addition, excellent agreement with the VISRAD analysis is observed. In the following discussion, the results of this rigorous analysis of a phenolic-nylon ablator will be more closely examined and a comparison made with the carbon-phenolic ablator.

The Effects of Simplifications in Property Models Upon Radiation Heating Prediction

Using phenolic nylon and air mixture properties for the injected gases, analyses were performed for each of the reference cases assuming both binary and multicomponent diffusion. The analysis of the effects of viscosity, thermal conductivity and heat capacity models were performed assuming binary diffusion. The results of these investigations are presented in the following section.

Heating Rate Comparison for Binary and Multicomponent Diffusion: Davy, *et al*. (Ref. 6.8), reported that for systems with large variations in molecular size,

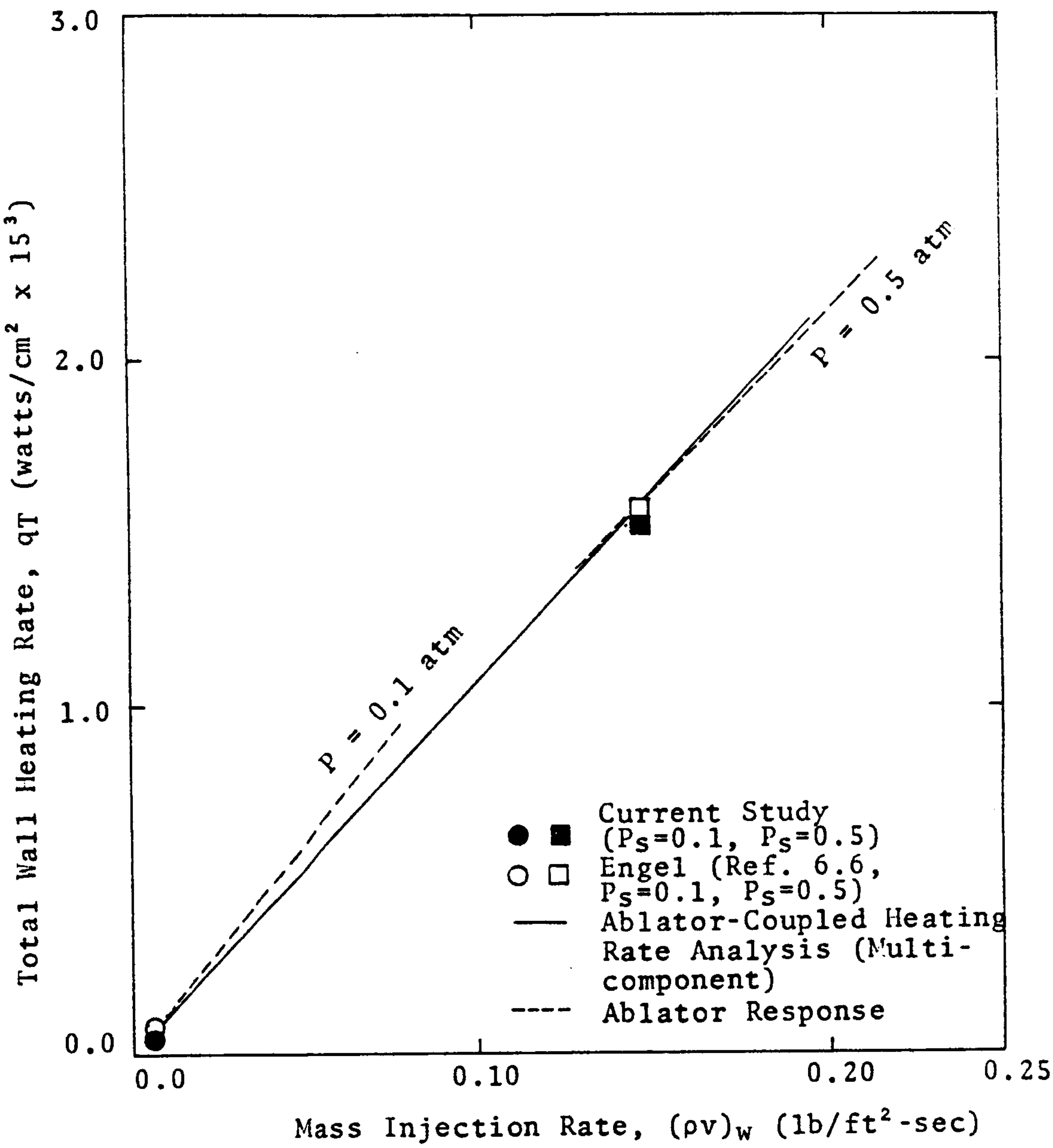

Figure 6.2. Ablator-Coupled Heating Rate Predictions for Phenolic-Nylon Ablator.

a binary coefficient characteristic of a large-small molecular interaction yielded the best results in predicting the multicomponent behavior. Therefore, the binary diffusion coefficient selected for the following comparison to multicomponent analyses was $H\text{-}C_2H_2$ (as computed from Equation 4.11). The heating rates and flight conditions pertinent to this comparison are presented in Table 6.3, and in Figure 6.3 the computed elemental distributions for the low and high blowing cases are shown for binary and multicomponent solutions. Referring to Table 6.3 the assumption of binary diffusion resulted in predictions of radiation heating rates which were in error by 16.8% in the case of low mass injection (Fig. 6.5A) and 2.1% for the high blowing case (Fig. 6.5B). The first observation to be made concerning these results is that the binary diffusion model selected for this comparison substantially over-predicts the diffusion velocities predicted by the more rigorous multicomponent analysis. It is further observed that the thickness of the diffusion zone is considerably less for the higher blowing rate. Although this effect can be partially attributed to the pressure differences, the principle cause is felt to be the differences in

TABLE 6.3

COMPARISON OF HEATING RATE PREDICTIONS FOR BINARY AND MULTICOMPONENT ANALYSES

Case Number	ρ_∞ (lb/ft)	U_∞ (ft/sec)	$\frac{(\rho v)_w}{(\rho v)_\infty}$	T_s (^oK)	P_s (atm)	Diffusion Model	Injectant Properties C_p	μ	k	δ (cm)	Wall Heating Rates (watts/cm^2) Convective	Radiative
4	2.85×10^{-6}	50,000	0.05	12,998	0.1	MCD*	PN**	PN	PN	10.85	120	340
5	2.85×10^{-6}	50,000	0.05	12,998	0.1	Binary	PN	PN	PN	10.85	120	397
6	1.45×10^{-5}	50,000	0.20	14,382	0.5	MCD	PN	PN	PN	13.93	0.3	2022
7	1.45×10^{-5}	50,000	0.20	14,382	0.5	Binary	PN	PN	PN	13.93	0.3	2064

*(MCD) Multicomponent diffusion
**(PN) Phenolic Nylon

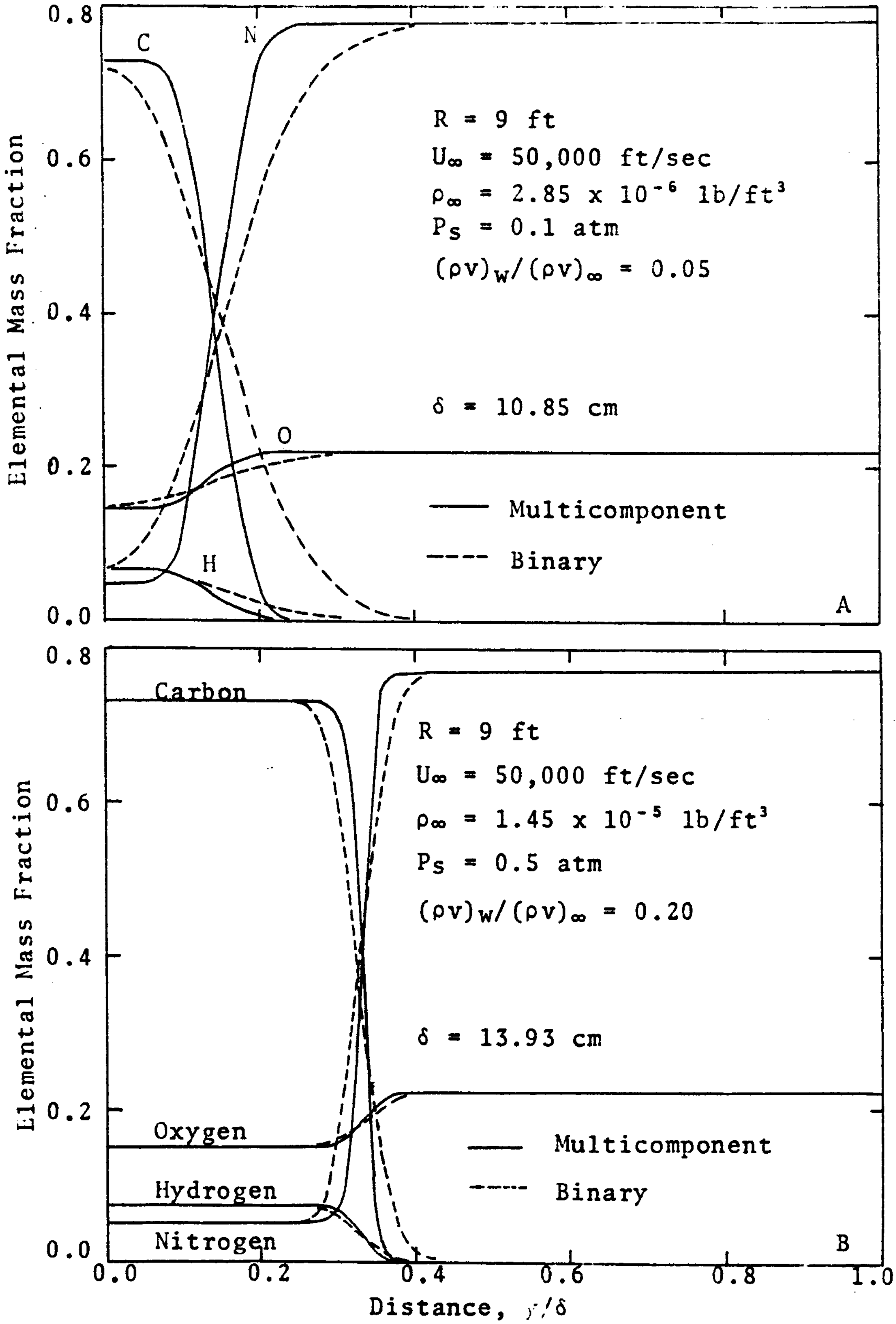

Figure 6.3. Comparison of Elemental Profiles Obtained From Binary and Multicomponent Diffusion Calculations.

the corresponding velocity profile. It has been observed that for higher blowing rates, the velocity profile changes more abruptly through the stagnation region, thereby reducing the zone in which the diffusion velocities contribute to the total mass flux.

The species mass fractions corresponding to the previously given elemental solutions are presented in Figures 6.4, 6.5, 6.6 and 6.7. These figures include comparisons between binary and multicomponent behavior for the principle species. For the low blowing case presented in Figures 6.4 and 6.5, considerable differences in the predicted compositions are observed. In contrast, the differences predicted for the high blowing case are quite small (Figs. 6.6 and 6.7).

From these observations, it can be concluded that for the high blowing rate case, the choice of diffusion models has very little influence upon the wall heating rates. From the low blowing rate case it is concluded that a more precise description of the diffusion process is needed for accurate heating rate predictions. This result contradicts the

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*A more precise description could be obtained by performing uncoupled studies with the multicomponent diffusion analysis developed in this study.

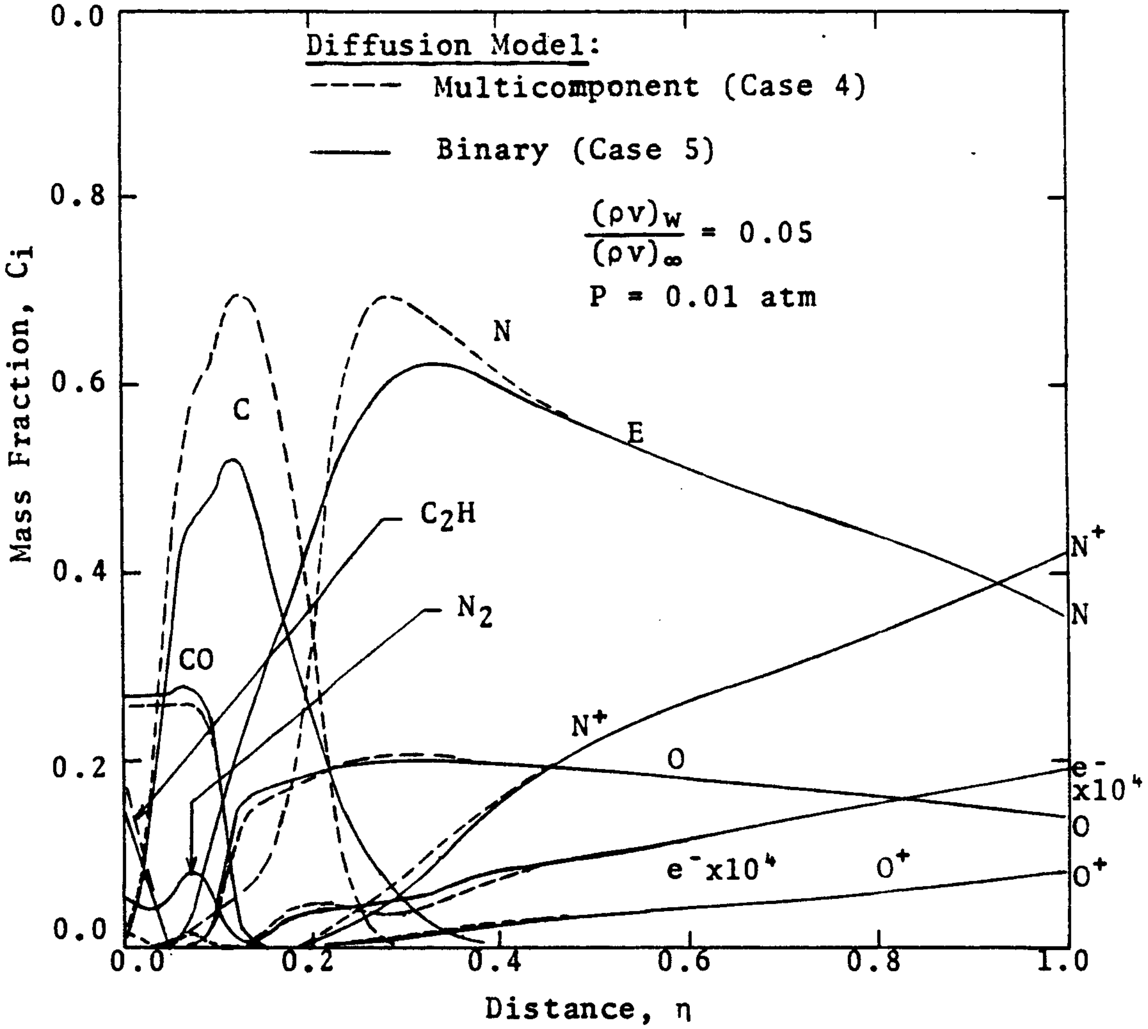

Figure 6.4. Composition Profiles For Air and Major Ablation Species.

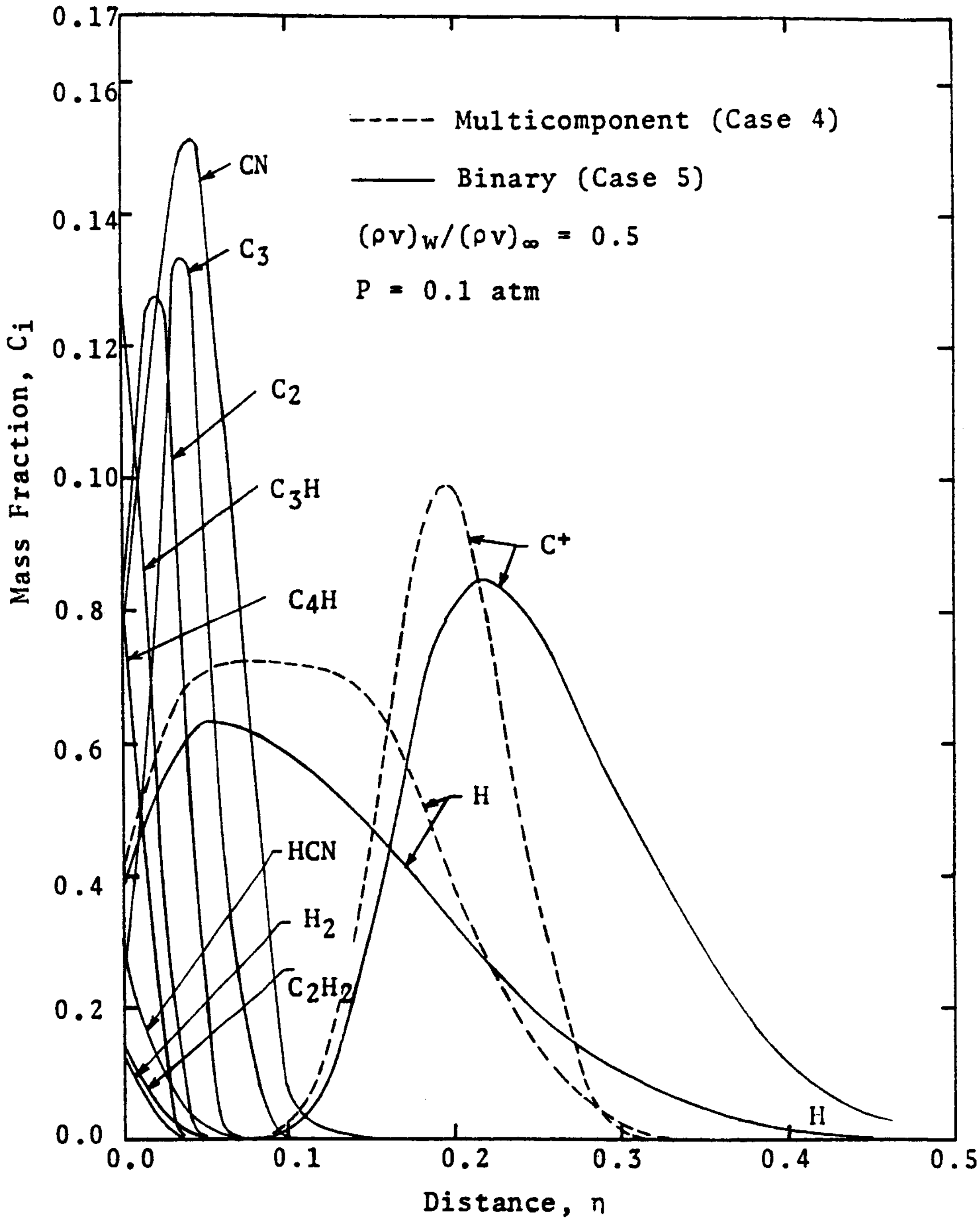

Figure 6.5. Composition Profiles for Minor Ablation Species.

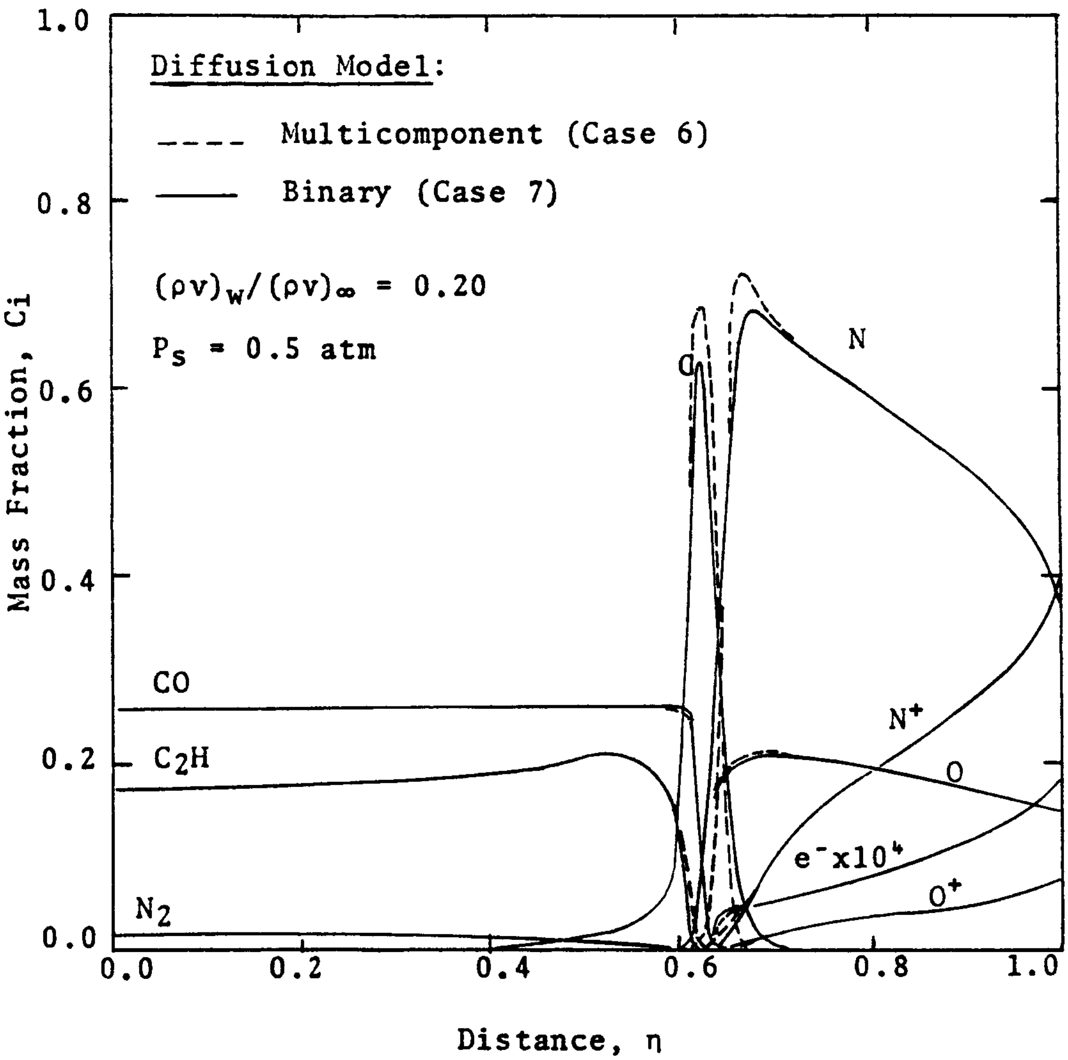

Figure 6.6. Composition Profiles for Air and Major Ablation Species.

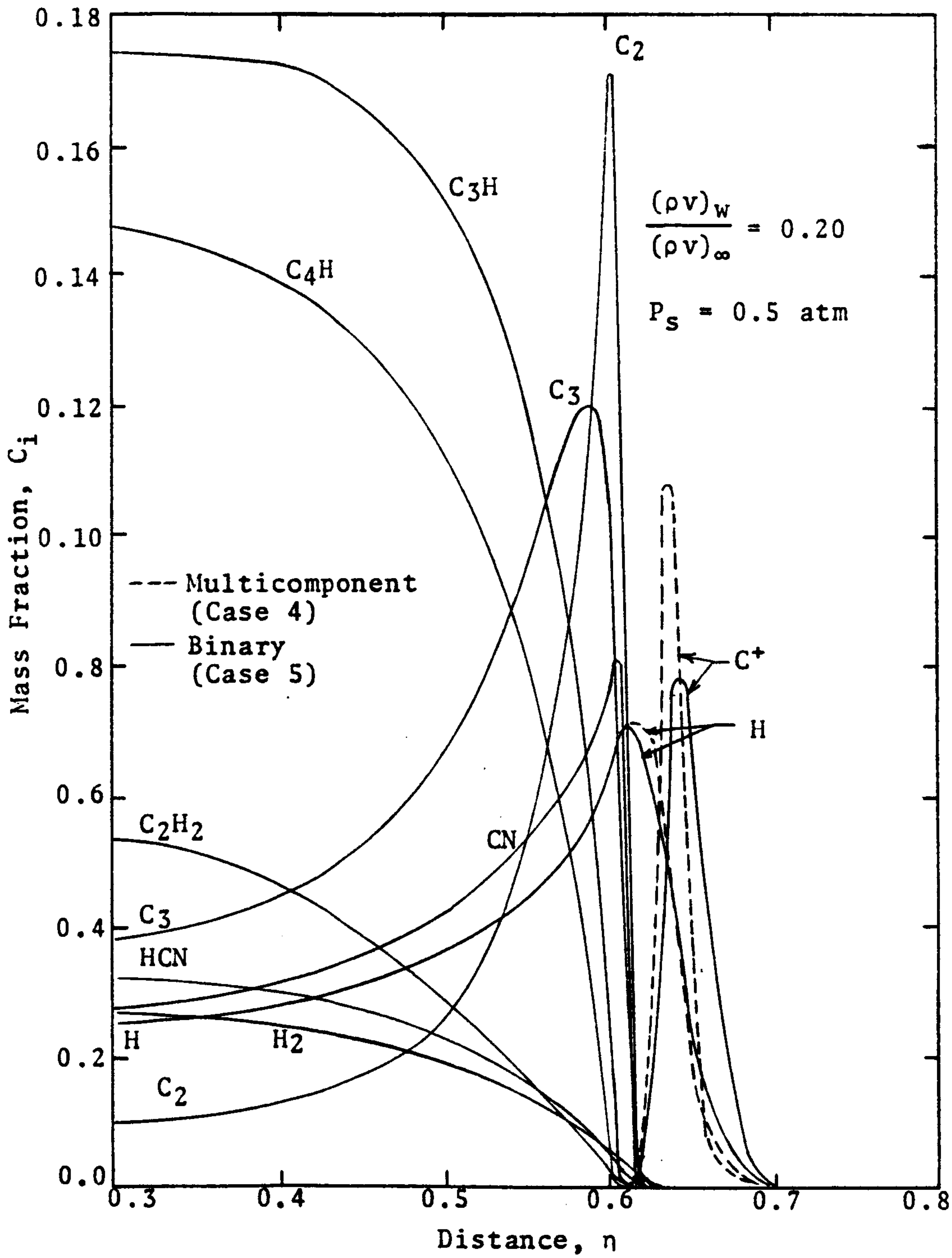

Figure 6.7. Composition Profiles for Minor Ablation Species.

observation by Rigdon, "that the choice of binary diffusion was not critical" (Ref. 6.2). However, the statement is applicable for high blowing situations such as those on which his statement was based.

It is noted that for the low blowing and correspondingly low pressure case (0.1 atm), the error in radiative heating is of little consequence since the heating rate itself is an order of magnitude less than the heating rate observed for the 0.5 atmosphere case. Recalling Figure 6.2 it is noted that as the heating rate increases to higher and more significant values the mass injection rate correspondingly advances. The ablator thus responds in such a manner as to decrease the inaccuracies in heating rate predictions which are brought about by the simplified diffusion model.

Comparisons of Heating Rate Predictions Using Ablation Product-Air and Pure Air Transport and Thermodynamic Properties

In the previous section it was noted that for large blowing rates, the selected binary diffusion coefficient gave a good approximation of the diffusion process. In spite of the differences (16.8%) in heating rate predictions encountered for the low blowing rate case, it is felt that this model is suitable for studies of the effects of assuming different transport and thermodynamic property models. Therefore, for computational convenience, the same binary coefficient was employed for the results of this section. Also, a preliminary analysis revealed that the effect of using air viscosity was negligible (less than 1.0%) with respect to heating rate predictions. Nevertheless, this property was computed in all cases to correspond to the actual composition of the air and ablation product mixture.

Comparisons were made at both the high and low blowing conditions to determine effect on heating rates of assuming air heat capacity and thermal conductivities for the injected ablation products. For the high blowing case, the effect of using only the thermal conductivity of air and maintaining the proper value for the remaining ablation product thermodynamic and transport properties was also examined. All of these results are summarized in Table 6.4. In Figure 6.8 and 6.9 comparisons are made between the temperature and radiative flux divergence profiles resulting from these assumptions for the high and low blowing cases.

TABLE 6.4

COMPARISON OF HEATING RATE PREDICTIONS OBTAINED BY ASSUMING AIR PROPERTIES FOR INJECTED SPECIES

Case Number	ρ_∞ (#/ft^3)	U_∞ (ft/sec)	$\frac{(\rho v)_w}{(\rho v)_\infty}$	T_s (^{o}K)	P_s (atm)	Diffusion Model	Injectant Properties c_p	μ	k	δ (cm)	Wall Heating Rate (watts/cm^2) Convective	Radiative
5	$2.85\text{x}10^{-6}$	50,000	0.05	12,998	0.1	Binary	PN*	PN	PN	10.85	120	397
8	$2.85\text{x}10^{-6}$	50,000	0.05	12,998	0.1	Binary	Air	PN	Air	11.38	44	372
7	$1.45\text{x}10^{-5}$	50,000	0.20	14,382	0.5	Binary	PN	PN	PN	13.93	0.3	2064
9	$1.45\text{x}10^{-5}$	50,000	0.20	14,382	0.5	Binary	PN	PN	Air	13.90	1.2	2104
10	$1.45\text{x}10^{-5}$	50,000	0.20	14,382	0.5	Binary	Air	PN	Air	15.95	0.5	1964

*Phenolic Nylon

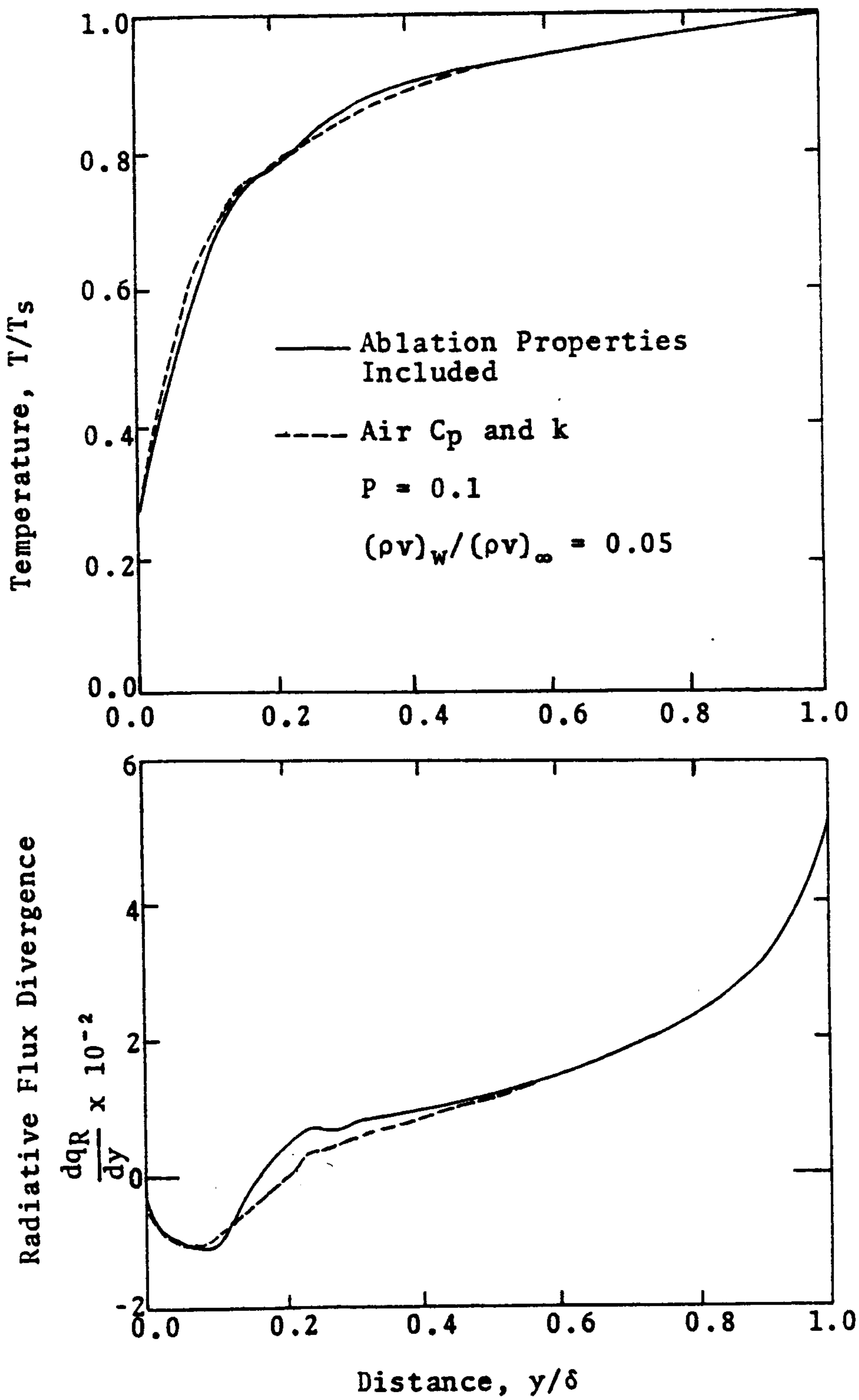

Figure 6.8. Temperature and Flux Divergence Profiles for Various Property Models.

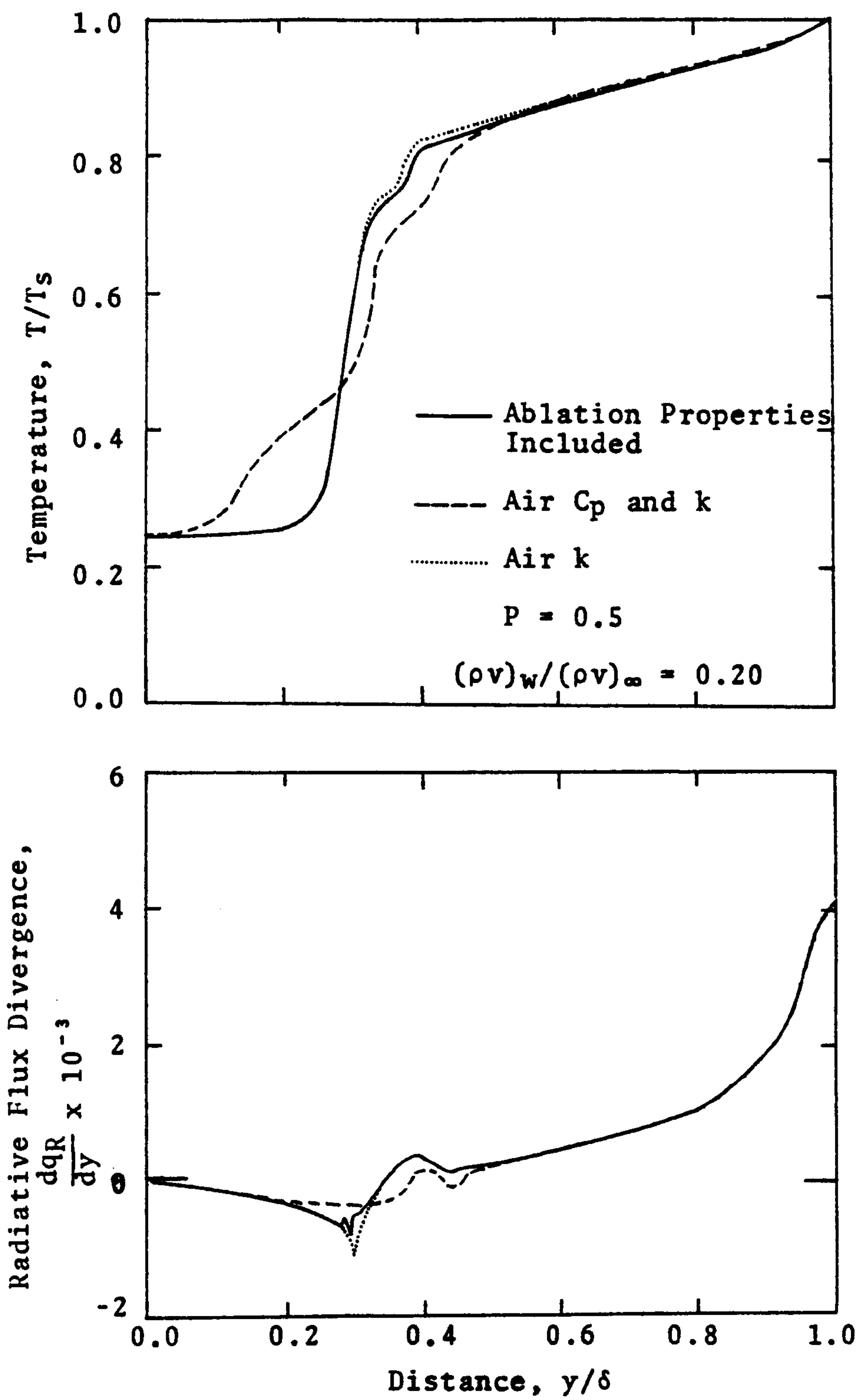

Figure 6.9. Temperature and Flux Divergence Profiles for Various Property Models.

For the low pressure, low mass injection case (Fig. 6.8), the radiative heating was underpredicted by 4.8% by using the air properties. Although the air properties resulted in an increase of approximately 120% in wall temperature gradient, the predicted convective heating rate was reduced by 63.3%. In comparison to the total heating this error only amounts to 14.7%. In Figure 6.10, the ratios of the properties of phenolic nylon and air mixtures to the corresponding properties of pure air are given for the cases considered. From this figure, it is noted that at the wall temperature of 3450°K, the actual thermal conductivity is approximately six times the corresponding pure air property, thus explaining the observed variation in convective heating rates.

For the higher blowing case (Fig. 6.9), very little change is observed in the temperature and flux divergence profiles as a result of using air thermal conductivity for the injected gases. The result is attributed to the fact that the conduction effects are restricted to a thin region around the stagnation point. The variation in predicted radiative heating rates resulting from this assumption was only 1.9%.

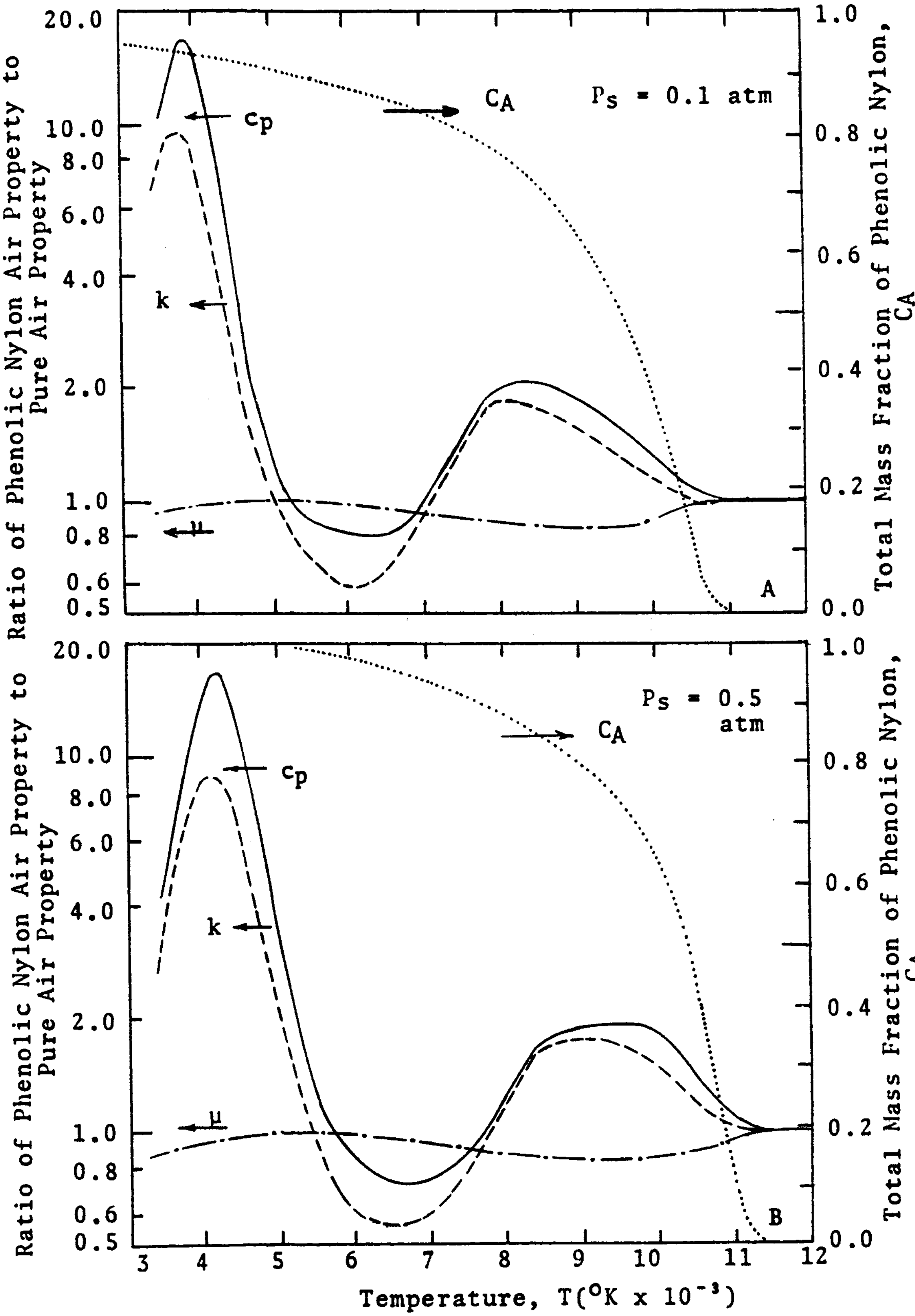

Figure 6.10. Comparison Between Phenolic Nylon and Air Mixture Properties to Those of Pure Air.

In comparing the effect of using air heat capacity for the ablation products, it is noted that extensive differences* appear in both the temperature and radiative flux divergence profiles. In spite of these observations, the predicted radiation heating rates varied only by 4.8%.

In this case the assumption of air properties resulted in an increase in shock stand-off distance from 13.93 cm to 15.95 cm (a 14.5% increase). This effect accounts for the fact that while the outer temperatures for the air properties case were generally lower (tending toward lower heating rates), the zone of more intense radiation (the high temperature air) was more extensive. Since these effects have confounded the results, a general conclusion concerning the importance of assuming the correct heat capacity for the injected species cannot be made. However, for both of the cases considered, the reduction of temperature which occurs in the ablation layer when the proper heat capacity is included, is attributed to the resulting increase in heat capacity. In fact, as shown in

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*It should be pointed out that the flux divergence profile appearing in Figure 6.11 has been scaled down by a factor of ten as compared to the low pressure case shown in Figure 6.10.

Figure 6.10, the heat capacity of phenolic-nylon at the wall temperature (3450°K) is approximately 17 times greater than air for the same temperature. Due to the extensive varitions in temperature and flux divergence that were observed in this comparison (Fig. 6.9), it is concluded that the use of air heat capacity for injected species can contribute to significant errors in heating rate predictions.

The Effectiveness of Phenolic Nylon Ablators in Reducing Radiative Heat Transfer to the Wall

In the following discussion an attempt will be made to compare the performance of the phenolic-nylon ablator examined in this analysis with the performance of carbon-phenolic ablators reported in References 6.1 to 6.4. However, little agreement has been reported in comparisons among investigations of the carbon-phenolic ablator. It is felt that the apparent lack of agreement is due to two major causes: (1) ill-suited comparisons (e.g., values obtained from widely varying flight conditions and body geometry) and (2) oversimplified radiation models. Consequently, an effort was made to select and compare only data from consistent flight conditions and body radii. As a consequence, no comparisons were available for the low pressure (P_s = 0.1) case. However, several values were reported in the range of the higher pressure (P_s = 0.5) case. A comparison among these results is shown in Figure 6.11. The value reported by Smith, et al. (Ref. 6.4) is considered to be somewhat in error due to the fact that line radiation contributions from atomic carbon and hydrogen were excluded in that analysis. Similarly, the results of Wilson (Ref. 6.1) include only continuum radiation. In comparing the performance of the phenolic-nylon ablator examined in the current study to that of the carbon-phenolic ablator it is desirable for an ablator-coupled mass injection rate to be also used for the latter system. Unfortunately this information is not available. However it is reasonable to assume that the ablator response for these two systems is similar; therefore a comparison can be made at the mass injection rate of 20%. On the basis of this comparison it appears that the phenolic-nylon ablator is approximately 5% less effective than the carbon phenolic ablator.*

*Under the imposed flight conditions.

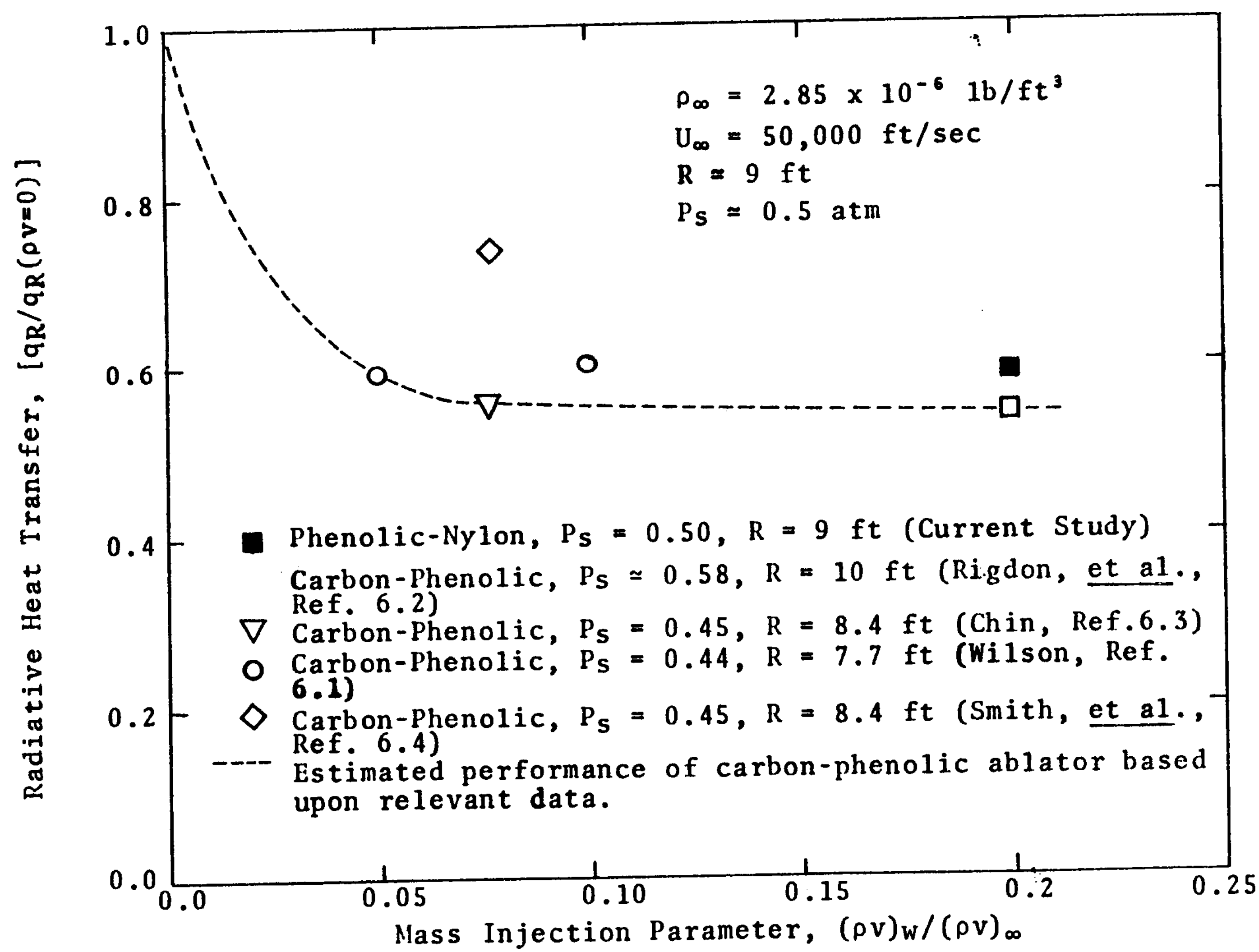

Figure 6.11. Comparison Between Effectiveness of Phenolic-Nylon and Carbon-Phenolic Ablators.

Further Observations

Irregularities in predicted temperature profiles: Since the intermediate plateaus in the temperature profiles are present for all cases considered, their presence is attributed to radiation phenomena. Further evidence of the radiation origins of this behavior is the fact that the plateaus are less pronounced for the low pressure cases where radiation is substantially less. Upon examining the species distribution corresponding to these cases (Figs. 6.5, 6.6, 6.7 and 6.8) it is observed that the spacial location of the large peak in atomic corresponds exactly to the location of the intermediate temperature plateaus. The local increase in the absorption of the ablation layer due to the presence of this species is thus considered cause of the intermediate plateaus in the temperature distributions.

Thermal Diffusion Effects: Throughout the preceding heating rate analysis, the contributions of thermal diffusion have been neglected. Due to the extremely high values of the radiation heat transport, large variations (as much as a factor of six) in thermal conductivities were observed to have only slight effects upon the radiation heat flux (a maximum of 4.8%). Furthermore, in the process of examining the effects of binary and multicomponent diffusion on radiation heating predictions, large variations in the diffusive behavior were observed. In spite of these variations a relatively small effect upon the heating rate was detected. It is well known from irreversible thermodynamics that the cross effects--in this case the Soret and Dufour effects--are small with respect to the principle transport mechanisms. It would therefore appear that the thermal diffusion effects are indeed negligible. To further substantiate this reasoning, a *posteriori* assessment was made of the contribution to the mass fluxes resulting from the large temperature gradients encountered.* A conservative estimate revealed that the maximum Soret effect is at least an order of magnitude less than the significant species mass fluxes. On the basis of the foregoing observations, it is therefore concluded that the neglect of thermal diffusion effects is an appropriate assumption in the current analysis.

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*See Appendix I.

Incomplete Radiation Data: An examination of the molar compositions corresponding to the species distributions presented in Figures 6,5-6.8 reveals that the ablation species included in the radiation model (LRAD)* represent a large percentage of those actually present. Overall, the minimum total molar percentage of the included species was 81.5% (Case 6). Furthermore, this percentage was seen to increase up to the stagnation point where a value of 93.7% was observed. From the flux divergence profile given in Figure H-4 it is noted that the major portion of the radiative absorption in the ablation layer occurs in the region immediately behind the stagnation point where the excluded species are present in the lowest concentration.

Summary

An investigation of the performance of a phenolic-nylon ablator has been made for flight conditions characteristics of return from planetary flight. The conclusions and recommendations arising from the results of this study are presented in the following chapter.

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*The excluded species, for which no radiation data exists are C^+, CN, C_2H_2, C_3H, C_4H, and HCN.

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CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

Based upon the results of this research the following conclusions are drawn:

1. The binary diffusion can yield accurate heating rate predictions at all blowing rates provided the appropriate binary coefficient is employed.

2. For low mass injection, the choice of the appropriate binary diffusion coefficient is critical in determining the proper wall heating rate.

3. For large mass injection rates (>20%), typical of those occuring during peak heating, the principal transport mechanisms (i.e., diffusion, conduction, and viscous transport) contribute very little (<5%) to the heat transfer process.

4. For low mass injection (≤ 0.05) characteristic of low heating rates, thermal conduction significantly contributes to the heat transfer process.

5. Since heat capacity affects temperatures throughout the flowfield, this thermodynamic property

must be properly determined or significant errors in heat rate predictions will be computed.

6. For the flight conditions examined the 40% nylon-60% phenolic resin ablator is slightly less effective in blocking radiative heating (~5%) than the carbon-phenolic ablator which it was compared.

Recommendation for Design Calculations

Transport Properties: It has been observed in this study that for the higher heating rates (~20%) and correspondingly higher mass injection rates, the flowfield is inviscid except for a thin region at the stagnation point. Consequently, these heating rate predictions were insensitive to variations in transport properties (including diffusion coefficients). Although heating rates were affected by variations in transport properties at the low mass injection conditions, it was noted that the corresponding heating rates were an order of magnitude less than those anticipated during peak heating. Inaccuracies in heating predictions at these conditions are therefore of little consequence in determining overall surface removal for the entire trajectory. It is therefore recommended that for computational convenience simplifed transport models (i.e., air) be employed in design calculations relating to re-entry from planetary missions.

Heat Capacity: In this study heat capacity has been observed to affect temperature profiles throughout the flowfield. Therefore, it is recommended that this property be properly determined for the existing chemical system.

Recommendations for the Improvement of the SLAB Program

The major difficulty in the use of the SLAB program is that of maintaining the proper stepsize distribution. Although a stepsize control subroutine is employed in this analysis, it is quite common for the temperature profile to shift from one iteration to the next to such an extent that the current stepsize distribution is inadequate and has to be changed by hand. If this change is not made then instability occurs and the solution wanders off into oblivion. To circumvent this difficulty it is recommended that more steps be used in the analysis. For fear of further extending the required computer time, the addition of more steps was not attempted. In retrospect, it is felt that the overall analysis would be shorter since little or no time would be spent in recovering from instabilities.

An examination of the typical results obtained from this analysis reveals that the elemental profiles are constant over a large portion (80-90%) of the flowfield. In view of this fact, considerable time could be saved by internally establishing during the first iteration a table of equilibrium compositions of pure air and of the pure ablation products. In subsequent iterations it would then only be necessary to perform equilibrium calculations in the diffusion zone. In this manner, the computer time possibly could be reduced by as much as sixty to eighty percent.

NOMENCLATURE

Symbol	Description	Units
A_{ij}	Element ratio (defined in Appendix A)	
C_d	Drag coefficient	none
C_f	Friction factor	none
C_h	Heat transfer coefficient	none
C_p	Total heat capacity (defined by Equation 3.41)	FL/MT
C_{pf}	Frozen heat capacity, C_iC_{pi}	FL/MT
C_{pi}	Heat capacity of species i	FL/MT
C_i	Mass fraction of species i	none
C_j	Mass fraction of element j	none
C_p	Total molar heat capacity (Eq. 4.32)	FL/mole T
C_{pi}	Molar heat capacity of species i	FL/mole T
$\bar{D}$	Reference diffusion coefficient (Eq. 2.23)	L^2/t
D_{ij}	Binary diffusion coefficient	L^2/t
$\tilde{D}_j$	Effective elemental diffusion coefficient	L^2/t
D_i	Effective diffusion coefficient	L^2/t
D_i^T	Thermal diffusion coefficient	M/Lt

Symbol	Description	Units
D_{ij}	Multicomponent diffusion coefficient	L^2/t
e_{ij}	Mass fraction of element j in compound i (Appendix A)	none
f'	Velocity function $\left(\frac{df}{dn}\right)$	none
F_i	Diffusion factors (Eq. 2.23)	none
g_c	Gravitational constant	ML/Ft^2
H	Total enthalpy, $H = h + \frac{v^2}{2g_c}$	FL/M
h	Static enthalpy, $h - C_i h_i$	FL/M
h_i	Enthalpy of species i	FL/M
H_T^o	Molar enthalpy at temperature T	FL/mole
I_j	Total mass flux of element j	M/L^2t
J_i	Diffusive mass flux of species i	M/L^2t
$\tilde{J}_j$	Diffusive mass flux of element j	M/L^2t
k	Total thermal conductivity (Eq. 3.42)	F/tT
k_f	Frozen thermal conductivity (Eq. 4.5)	F/tT
k_b	Bulk thermal conductivity (of char)	F/tT
ℓ	Number of elements	none
m	Mass	M
m_i	Mass of particle i	M
M	Molecular weight	M/mole
M_i	Molecular weight of species i	M/mole

Symbol	Description	Units
$\tilde{M}_j$	Atomic weight of element i	M/mole
n	Number density	particles/ L^3
P	Pressure	F/L^2
P_r	Prandtl number, $C_p\mu/k$	none
q_r	Radiative heat flux	F/Lt
q_r^+	Total radiative heat flux at the wall	$\dot{F}$/Lt
R	Principal body radius	L
$\mathbb{R}$	Ideal gas constant	F/mole T
r_i	Homogeneous reaction term	M/TL^3
Re_s	Reynolds number, $\rho_s, U_\infty, R/\mu_s$	
s_i	Sublimation rate	M/TL^3
S_i	Surface mass generation	M/TL^3
T	Temperature	T
T_{ij}^*	Reduced temperature (Eq. 4.13)	none
u	Tangential velocity	L/t
v	Normal velocity	L/t
U_∞	Normal free stream velocity	L/t
Y_i	Mole fraction of species i	none
δ	Shock standoff distance	L
$\tilde{\delta}$	Transformed standoff distance (Eq. 3.93)	none
ε	Difference between body and shock angles (See Fig. 3.1)	radians

Symbol	Description	Units
η	Dorodnitzn variable	none
θ	Body angle (See Fig. 3.1)	radians
κ	Local body curvature	1/L
$\tilde{\kappa}$	1+ky	none
μ_i	Viscosity of species i	M/Lt
μ	Mixture viscosity	M/Lt
ν	Number of species	none
ρ	Density	M/L^3
ρ_i	Partial density of species i	M/L^3
ρ_g	Density of the gas phase	M/L^3
ρ_o	Density of the virgin plastic	M/L^3
$\bar{\rho}$	Density ratio across the shock	none
σ	Collision diameter	L
k_c	Stefan-Boltzmann constant 5.6697×10^{-8} watts/m^2 $^\circ K^4$	F/tLT^4
ϕ	Shock angle	Radians
$\omega_{i(1,1)}$	Chemical generation term	M/L^3t
Ω_{ij}	Collision integral for diffusion coefficients	none

Subscripts

i	Species i	
w	Wall quantities	
0	Stagnation line quantities	

Symbol	Description	Units
∞	Free-stream conditions	
S	Quantities immediately behind shock	

Superscripts

0	Standard state quantity	
-	Evaluated on char side of ablator interface	
+	Evaluated on flowfield side of ablator interface	

APPENDIX A

TRANSFORMATION OF SPECIES CONTINUITY EQUATIONS TO ELEMENTAL CONTINUITY EQUATIONS

The elemental mass distribution within a single chemical component can be easily determined from the atomic weights of the elements present, $\tilde{M}_j$; the molecular weight of the compound, M_i; and the chemical formula. For example, the weight fractions of H in H_2O is 2/18 and 0 is 16/18. Mathematically this is expressed as follows:

$$e_{ij} = \frac{A_{ij}\tilde{M}_j}{M_i} = \text{(the mass of element j per unit mass of compound i)} \quad \text{(A-1)}$$

where A_{ij} is simply the moles of element j per mole of compound i. In the above example $A_{H_2O,H} = 2$ and $A_{H_2O,O} = 1$.

The elemental mass distribution within a mixture of chemical species can be determined from the species mass distribution by multiplying each component mass fraction by the corresponding elemental distribution and summing over all species as follows:

$$\tilde{C}_j = \sum_{i=1}^{\nu} e_{ij}C_i = \text{(mass fraction of element j)} \quad \text{(A-2)}$$

where C_i is the mass fraction of component i and ν is the number of species.

The elemental continuity equations can be derived from the species continuity equations (Eqs. 3.15) in the previous manner. The latter equations are written as follows:

$$\rho v \frac{dC_i}{dy} = - \frac{dJ_i}{dy} + \omega_i \tag{A-3}$$

Multiplication of each equation by the corresponding elemental distributions and summing over the species gives:

$$\rho v \frac{d\tilde{C}_j}{dy} = - \frac{d}{dy} \sum_{i=1}^{\nu} e_{ij} J_i + \sum_{i=1}^{\nu} e_{ij} \omega_i \qquad j=1,\ldots, \tag{A-4}$$

where is the total number of elements.

It is convenient to define $\tilde{J}_j$, an elemental mass diffusion flux as follows:

$$\tilde{J}_j = \sum_{i=1}^{\nu} e_{ij} J_i = \tilde{M} \sum_{i=1}^{\nu} \frac{A_{ij} J_i}{M_i} \tag{A-5}$$

Substituting Equation A-5 into Equation A-4, and noting that the total mass of any element is unchanged due to chemical reactions the elemental continuity equation can be written as follows:

$$\rho v \frac{d\tilde{C}_j}{dy} = - \frac{d\tilde{J}_j}{dy} \tag{A-6}$$

With the exception of the generation term, Equation A-6, is now of the same form as Equation A-3, the species continuity equation.

When the mass flux J_i appearing in Equation A-3 can be represented with binary diffusion (Fick's Law, Eq. 3.22), the elemental flux can be determined in the following manner. From Equation 3.22 and the definition of Equation A-5,

$$\tilde{J}_j = \sum_{i=1}^{\nu} e_{ij} \quad -\rho \mathcal{D}_{12} \frac{dC_i}{dy} \tag{A-7}$$

or,

$$\tilde{J}_j = - \rho \mathcal{D}_{12} \frac{d}{dy} \sum_{i=1}^{\nu} e_{ij} C_i \tag{A-8}$$

Substituting Equation A-2 gives

$$\tilde{J}_j = - \rho \mathcal{D}_{12} \frac{d\tilde{C}_j}{dy} \tag{A-9}$$

This relationship can be substituted directly into the Elemental Continuity Equations (Eqs. A-6) to describe the elemental distribution of a gaseous chemical system having a common diffusion coefficient ($\mathcal{D}_{12}$).

APPENDIX B

DERIVATION OF TOTAL THERMAL CONDUCTIVITY AND HEAT CAPACITY EXPRESSIONS

In this appendix, the expressions describing the total thermal conductivity and the total heat capacity are derived from a rearrangement of the.energy equation (Eq. 3.39). The development of these expressions is performed to demonstrate that the additional mechanisms (as opposed to the frozen properties) due to the existence of chemical reactions. It is shown that these effects are accounted for by terms contained in the energy equation which are not normally associated with these properties. The energy equation can be expressed as follows (Eq. 3.39):

$$\rho v C_p \frac{dT}{dy} = \frac{d}{dy}\left(k_f \frac{dT}{dy}\right) - \rho v \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} - \rho v^2 \frac{dv}{dy} - \frac{d}{dy} \sum_{i=1}^{\nu} h_i J_i - \frac{dq_R}{dy} \qquad \text{(B-1)}$$

The mass flux (J_i) can be exactly represented by the following relationship:

$$J_i = - \rho D_i \, dC_i/dy \qquad \text{(B-2)}$$

where D_i, is an effective diffusion coefficient as described in Chapter II. Substituting Equation B-2 into the energy equation (Eq. B-1) and rearranging the following relationship is obtained.

$$\rho v \quad C_{p_f} \frac{dT}{dy} + \sum_{i=1}^{\nu} h_i \frac{dC_i}{dy} = \frac{d}{dy} \quad k_f + \rho \sum_{i=1}^{\nu} D_i h_i \frac{dC_i}{dy}$$

$$- \rho v^2 \frac{dv}{dy} - \frac{dq_R}{dy} \tag{B-3}$$

For chemical equilibrium $C_i = C_i\ (T, P, \tilde{C}_1, \ldots \tilde{C}_\ell)$, therefore we can write

$$\frac{dC_i}{dy} = \frac{\partial C_i}{\partial T} \frac{dT}{dy} + \frac{\partial C_i}{\partial P} \frac{dP}{dy} + \sum_{j=1} \frac{\partial C_i}{\partial \tilde{C}_j} \frac{d\tilde{C}_j}{dy} \tag{B-4}$$

Since $dP/dy = 0$ (Eq. 3.17), then

$$\frac{dC_i}{dy} = \frac{\partial C_i}{\partial T} \frac{dT}{dy} + \sum_{j=1} \frac{\partial C_i}{\partial \tilde{C}_j} \frac{d\tilde{C}_j}{dy} \tag{B-5}$$

Substitution of this equation into Equation B-3 gives,

$$\rho v \left[c_{p_f} + \sum_{i=1}^{\nu} h_i \frac{\partial C_i}{\partial T} \right] \frac{dT}{dy} + \rho v \sum_{i=1}^{\nu} h_i \sum_{j=1} \frac{\partial C_i}{\partial \tilde{C}_j} \frac{d\tilde{C}_j}{dy} =$$

$$\frac{d}{dy} \left[k_f + \rho \sum_{i=1}^{\nu} D_i h_i \frac{\partial C_i}{\partial T} \right] \frac{dT}{dy} + \frac{d}{dy} \sum_{i=1}^{\nu} D_i h_i \sum_{j=1} \frac{\partial C_i}{\partial \tilde{C}_j} \frac{d\tilde{C}_j}{dy}$$

$$- \rho v^2 \frac{dv}{dy} - \frac{dq_R}{dy} \qquad \text{(B-6)}$$

Due to the computational difficulties of determining the partial derivatives of concentration with respect to elemental concentration ($\partial C_i/\partial \tilde{C}_j$), previous investigators have neglected the additional terms containing these quantities. On the basis of a posteriori analysis, Wilson (Ref. 3.9) reported that only a slight contribution of these terms to the overall heat transport could be detected. Considering Wilson's observation, and the extent of the computational difficulties, the additional terms were neglected in the current analysis. Equation B-6 can then be written as,

$$\rho v C_p \frac{dT}{dy} = \frac{d}{dy} k \frac{dT}{dy} - \rho v^2 \frac{dv}{dy} - \frac{dq_R}{dy} \qquad \text{(B-7)}$$

$$\text{where } c_p = c_{p_f} + \sum_i h_i \frac{\partial C_i}{\partial T} = \text{total heat capacity} \tag{B-8}$$

$$\text{and } k = k_f + \rho \sum D_i h_i \frac{\partial C_i}{\partial T} = \text{total thermal conductivity} \tag{B-9}$$

It is observed that the total heat capacity (Eq. B-8) thus includes the effects of chemical heats of reaction as an additional mechanism for energy absorption. Furthermore, it is noted that the total thermal conductivity (Eq. B-9) accounts for an additional transport of energy through the diffusion of high energy molecules into regions of lower energy.

APPENDIX C

ESTIMATION OF COLLISION PARAMETERS FOR BINARY DIFFUSION COEFFICIENTS

The methods employed for the estimation of the ablation products (C_3, C_2H, C_3H, C_4H, and C^+) and air species (O, N, O^+, N, e^-) collision parameters are described in this appendix. A literature survey indicated that such data was unavailable for these species. Therefore, in the case of the ablation products, correlations were developed based upon similar types of species. For the air species, rigorous theoretical binary diffusion coefficients were reported from estimates of these parameters could be obtained.

Ablation Species (C_3, C_2H, C_3H, C_4H, and C^+

In Figures C-1 and C-2 the collision parameters of species similar to those of interest are plotted against molecular weight. In the case of the collision diameter σ (Figure C-1), excellent agreement is noted. From the data, the following correlation was obtained:

$$\sigma_i = 2.69 + 0.0514\ Mi \qquad \text{(C-1)}$$

This relationship was used to estimate the collision diameters of C_3, C_2H, C_3H and C_4H.

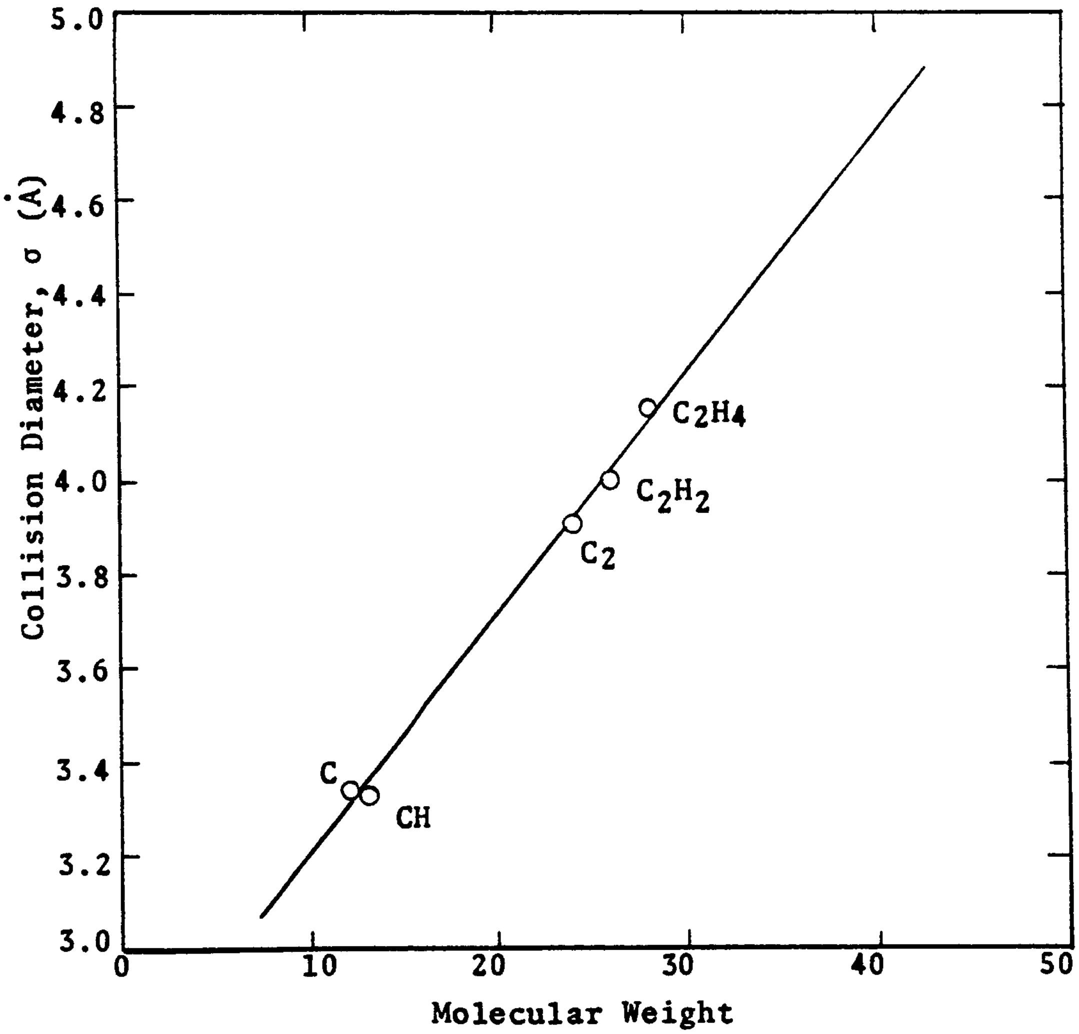

Figure C-1. Collision Diameter of Light Hydrocarbon Versus Molecular Weight (Ref. 4.5).

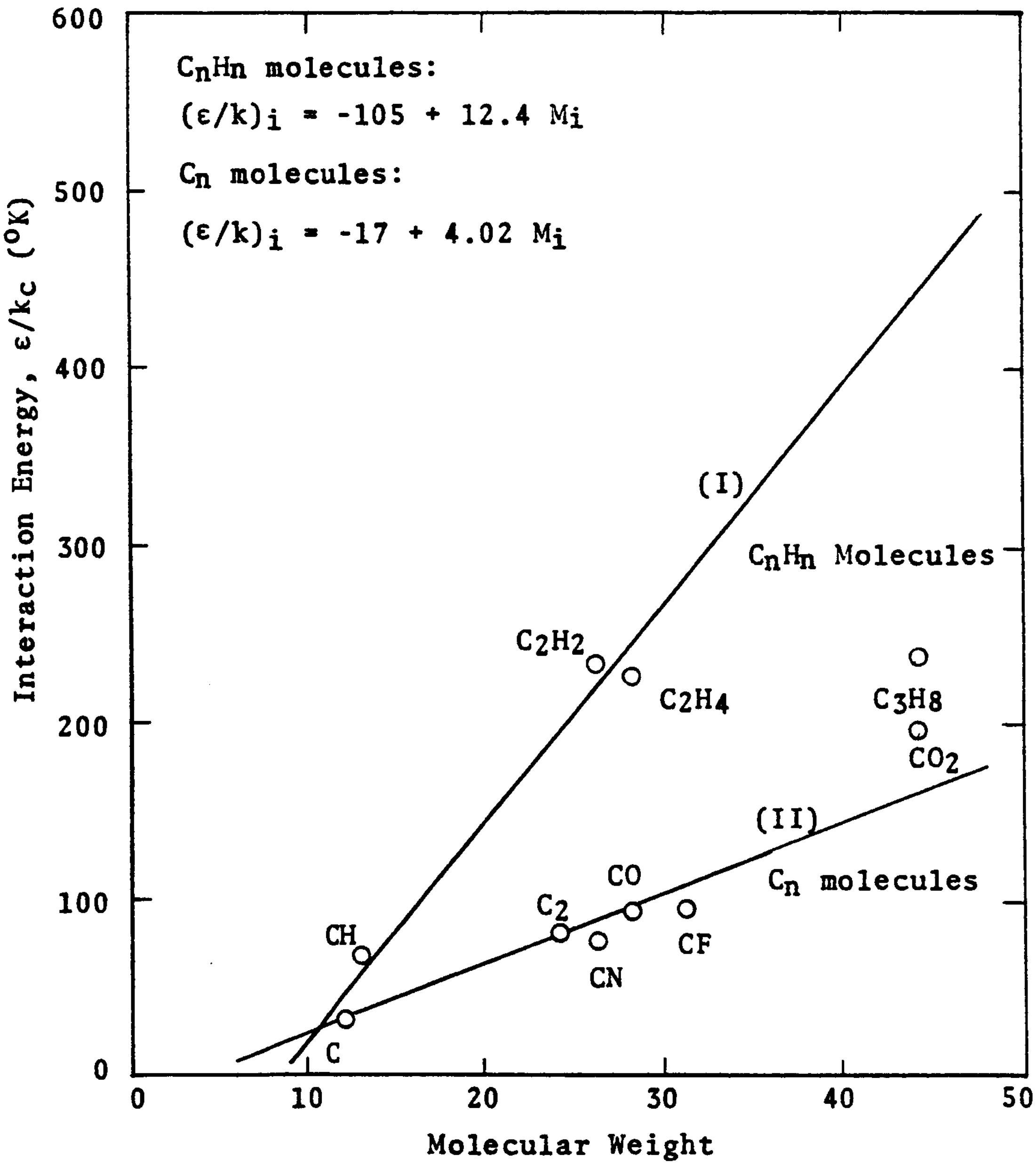

Figure C-2. Interaction Energy of Light Hydrocarbons Versus Molecular Weight (Ref. 4.5).

The correlations of interaction energy ε_i/k_c (Figure C-2) were obtained by grouping the C_nH_n compounds and the C_n compounds. The interaction energies of similar polyatomic molecules are also given to further support the validity of the C_n correlation (Curve II). The resulting correlations are given as follows:

C_nH_n Molecules (C_2H, C_3H, and C_4H):

$$\varepsilon_i/k_c = -105 + 12.4\ M_i$$

C_n Molecules (C_3):

$$\varepsilon_i/k_c = -17 + 4.02\ M_i$$

Air Species (O, N, O^+, N^+ and e^-)

The collision parameters for the high temperature air species were estimated from the binary diffusion coefficients reported by Yun, Wiessman, and Mason (Ref. 4.2) and Yos (Ref. 4.7). Some difficulty was encountered in attempting to simultaneously satisfy the theoretical data. Therefore, the correlations shown in Figure C-3 were obtained by arbitrarily weighting each interaction according to the frequency of its occurence over the temperature range of interest (3000-14000°K). In this manner a nearly exact fit was obtained for the most frequent interactions (atom-atom) while the least accurate fit was obtained for least frequent (ion-ion). The resulting correlations are shown in Figure C-3. The corresponding binary collision parameters are reported in Table 4.3. The electron (e^-) was assumed to exhibit the same diffusion characteristics as the parent dissociated atoms (N^+, O^+).

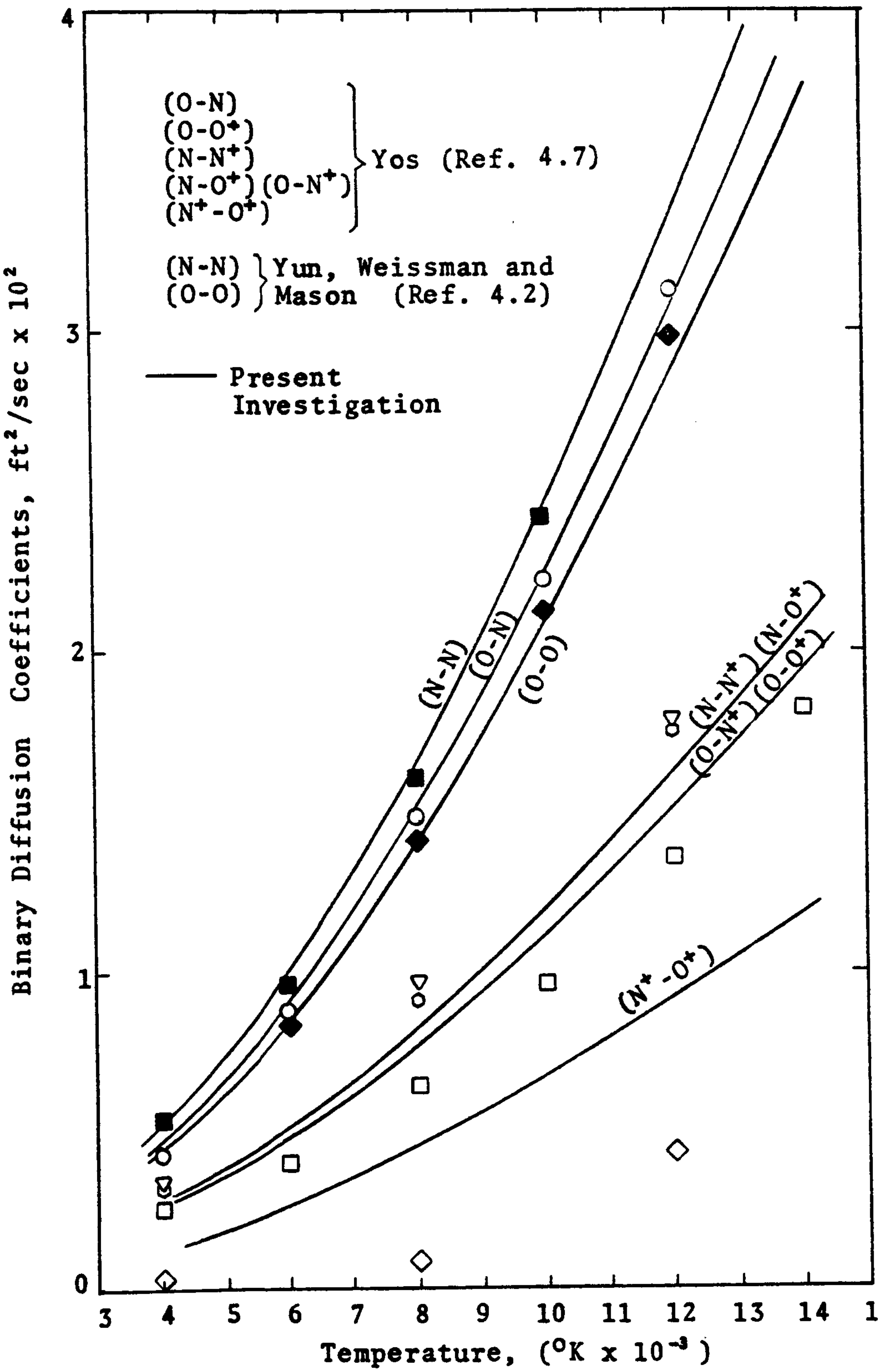

Figure C-3. Binary Diffusion Coefficients for the Constituents of Air at Atmospheric Pressure.

APPENDIX D

DETERMINATION OF POLYNOMIAL COEFFICIENTS FOR THERMODYNAMIC PROPERTIES

There are several procedures for obtaining the polynomial constants as required for the equations given in Table D-1. McBride, et al. (Ref. D-1), used a least squares technique which was simultaneously applied to all four of the thermodynamic functions. For the purpose of this study, the emphasis was placed upon the free energy fit rather than the properties in general. In the following paragraphs the procedure for determining these constants is explained.

From tabulated enthalpy functions as given in several reports (Refs. 4.12-4.17), the following polynomial was curve fit using a simple least squares analysis.

$$\frac{H_T^o - H_0^o}{RT} = B_1 + B_2T + B_3T^2 + B_4T^3 + B_5T^4 \qquad \text{(D-1)}$$

From Equation 4.22 the constants A_1 through A_5 were determined as shown below:

$$A_1 = B_1$$

$$A_2 = 2B_2$$

TABLE D-1

A SUMMARY OF RELATED POLYNOMIAL EQUATIONS FOR STANDARD THERMODYNAMIC PROPERTIES

Specific Heat

$$\frac{C_p^o}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4 \qquad \text{(A)}$$

Enthalpy

$$\frac{H_T^o}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \qquad \text{(B)}$$

Entropy

$$\frac{S_T^o}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4} + A_7 \qquad \text{(C)}$$

Free Energy

$$\frac{F_T^o}{RT} = A_1(1-\ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4$$

$$+ \frac{A_6}{T} - A_7 \qquad \text{(D)}$$

$$A_3 = 3B_3$$

$$A_4 = 4B_4$$

$$A_5 = 5B_5$$

The constant, A6, was computed separately from Equation 4.27:

$$A_6 = H_0^{o}/R = (\Delta H_f)_{T_{ref}} - (H_T^{o} - H_0^{o})_{T_{ref}} / R \tag{4.27}$$

where $(\Delta H\ )_{T_{ref}}$ = heat of formation at the reference temperature (298.16°K).

$(H_T^{o} - H_0^{o})_{T_{ref}}$ = Enthalpy (relative to absolute zero) at the reference temperature.

The value of A7 was determined as the constant difference between the tabulated free energy data and the remaining terms of the free energy polynomial as computed from the previously determined constants.

$$A_7 = A_1(1-\ln T) - \frac{A_2}{2} - \frac{A_3T^2}{6} - \frac{A_4T^4}{12} - \frac{A_5T^5}{20} - \frac{F_T^{o} - H_0^{o}}{RT} \tag{D-2}$$

In this report constants were evaluated at two temperature ranges for all species of interest and are listed in Table D-2. The ranges considered were 1000-7000°K and 5000-18000°K. The overlapping and extension of temperature ranges was necessary to overcome accuracy limitations at the extremes of the fit. The constants used for C_3H, C_4H, and HCN were taken from Duff (Ref. D-2) and are valid to 6000°K. Above this temperature these species do not exist in significant quantities at pressures of interest in the study.

TABLE D-2

POLYNOMIAL COEFFICIENTS FOR THERMODYNAMIC PROPERTY CORRELATIONS

Species	A1	A2	A3	A4	A5	A6	A7	T*
C+	0.2609E 01	-0.1393E-03	0.5959E-07	-0.1037E-10	0.6345E-15	0.2168E 06	0.3709E 01	L
	0.2528E 01	0.4869E-05	-0.7026E-08	0.1134E-11	-0.3476E-16	0.2168E 06	0.4139E 01	H
H	0.2500E 01	-0.8243E-06	0.6421E-09	-0.1720E-12	0.1457E-16	0.2547E 05	-0.4612E 00	L
	0.3934E 01	-0.1776E-02	0.6013E-06	-0.7819E-10	0.3482E-14	0.2547E 05	-0.8598E 01	H
N+	0.2727E 01	-0.2820E-03	0.1105E-06	-0.1551E-10	0.7847E-15	0.2254E 06	0.3645E 01	L
	0.2499E 01	-0.3725E-05	0.1147E-07	-0.1102E-11	0.3078E-16	0.2254E 06	0.4950E 01	H
O+	0.2491E 01	0.2762E-04	-0.1881E-07	0.3807E-11	-0.1028E-15	0.1879E 06	0.4424E 01	L
	0.2944E 01	-0.4108E-03	0.9156E-07	-0.5848E-11	0.1190E-15	0.1879E 06	0.1750E 01	H
E-	0.2500E 01	0.3440E-06	-0.1954E-09	0.3937E-13	-0.2573E-17	-0.7450E 03	-0.1173E 02	L
	0.2508E 01	-0.6332E-05	0.1364E-08	-0.1094E-12	0.2934E-17	-0.7450E 03	-0.1208E 02	H
C	0.2612E 01	-0.2030E-03	0.1095E-06	-0.1695E-10	0.8590E-15	0.8542E 05	0.4144E 01	L
	0.2141E 01	0.3219E-03	-0.5498E-07	0.3604E-11	-0.5564E-16	0.8542E 05	0.6874E 01	H
CN	0.3411E 01	0.4897E-03	0.1005E-06	-0.3473E-10	0.2361E-14	0.4745E 05	0.4746E 01	L
	0.3473E 01	0.7337E-03	-0.9088E-07	0.4847E-11	-0.1018E-15	0.5420E 05	0.4152E 01	H
CO	0.3254E 01	0.9698E-03	-0.2647E-06	0.3037E-10	-0.1177E-14	-0.1434E 05	0.4875E 01	L
	0.3366E 01	0.8027E-03	-0.1968E-06	0.1940E-10	-0.5549E-15	-0.1434E 05	0.4263E 01	H
C2	0.4443E 01	-0.2885E-03	0.3036E-06	-0.6244E-10	0.3915E-14	0.9787E 05	-0.1090E 01	L
	0.4026E 01	0.4857E-03	-0.7026E-07	0.4666E-11	-0.1142E-15	0.9787E 05	0.1090E 01	H
C2H	0.3485E 01	0.3563E-02	-0.1237E-05	0.1866E-09	-0.1013E-13	0.5809E 05	0.4784E 01	L
	0.5307E 01	0.8966E-03	-0.1378E-06	0.9251E-11	-0.2278E-15	0.5809E 05	-0.5288E 01	H

*Temperature Range L = 1000-6000°K, H = 6000-15,000°K

(continued)

TABLE D-2 (continued)

Species	A1	A2	A3	A4	A5	A6	A7	T*
C2H2	0.3891E 01	0.5717E-02	-0.1957E-05	0.2931E-09	-0.1585E-13	0.2590E 05	0.6520E 00	L
	0.6789E 01	0.1503E-02	-0.2295E-06	0.1534E-10	-0.3763E-15	0.2590E 05	-0.1539E 02	H
C3	0.4002E 01	0.3541E-02	-0.1318E-05	0.2064E-09	-0.1144E-13	0.9423E 05	0.2020E 01	L
	0.2213E 02	-0.1759E-01	0.5565E-05	-0.6758E-09	0.2825E-13	0.9423E 05	-0.1021E 03	H
C3H	0.3965E 01	0.6200E-02	-0.2265E-05	0.3717E-09	-0.2262E-13	0.6283E 05	0.3467E 01	L
	0.3965E 01	0.6200E-02	-0.2265E-05	0.3717E-09	-0.2262E-13	0.6283E 05	0.3467E 01	H
C4H	0.5874E 01	0.7403E-02	-0.2729E-05	0.4437E-09	-0.2637E-13	0.7605E 05	-0.4010E 01	L
	0.5874E 01	0.7403E-02	-0.2729E-05	0.4437E-09	-0.2637E-13	0.7605E 05	-0.4010E 01	H
HCN	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	L
	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	H
H2	0.3358E 01	0.2794E-03	0.9372E-07	-0.2948E-10	0.2141E-14	-0.1018E 04	-0.3548E 01	L
	0.3363E 01	0.4656E-03	-0.5127E-07	0.2802E-11	-0.4905E-16	-0.1018E 04	-0.3716E 01	H
N	0.2474E 01	0.9097E-04	-0.7814E-07	0.2218E-10	-0.1489E-14	0.5609E 05	0.4300E 01	L
	0.2746E 01	-0.3909E-03	0.1338E-06	-0.1191E-10	0.3369E-15	0.5609E 05	0.2872E 01	H
O	0.2670E 01	-0.1970E-03	0.7193E-07	-0.8901E-11	0.4002E-15	0.2915E 05	0.4504E 01	L
	0.2548E 01	-0.5952E-04	0.2701E-07	-0.2798E-11	0.9380E-16	0.2915E 05	0.5049E 01	H
N2	0.3221E 01	0.9878E-03	-0.2907E-06	0.3938E-10	-0.2000E-14	-0.1043E 04	0.4326E 01	L
	0.3727E 01	0.4684E-03	-0.1140E-06	0.1154E-10	-0.3293E-15	-0.1043E 04	0.1294E 01	H
O2	0.3316E 01	0.1151E-02	-0.3726E-06	0.6186E-10	-0.3666E-14	-0.1044E 04	0.5393E 01	L
	0.3721E 01	0.4254E-03	-0.2835E-07	0.6050E-12	-0.5186E-17	-0.1044E 04	0.3254E 01	H

*Temperature Range L = 1000-6000°K, H = 6000-15,000°K

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D-2. Duff, R. E. and S. H. Bauer, "Equilibrium Composition of the C/H System at Elevated Temperatures," Jour. Chem. Physics, Vol. 36, 1754 (1962).

APPENDIX E

DETERMINATION OF EQUILIBRIUM COMPOSITIONS

A free energy minimization approach was used in the current study to determine equilibrium species compositions. The minimization technique employed in the analysis is the method of undetermined multipliers and was originally presented by White, Johnson, and Dantzig (Ref. E-1). The present analysis, a subroutine (CHEMEQ) was developed through an extensive modification of a program based upon the above method and reported by Stroud and Brinkley (Ref. E-2). Prior to being used in both the SLAB and the SLAM programs, this subroutine was carefully tested and found to be predicting compositions which were in full agreement with other investigators. In Figure E-1, a comparison with other investigators is shown for the prediction of equilibrium air compositions. Excellent agreement is observed. Further verifications is noted in Figure 4.9 in a comparison of predicted values of reacting heat capacity (Eq. 4.32).

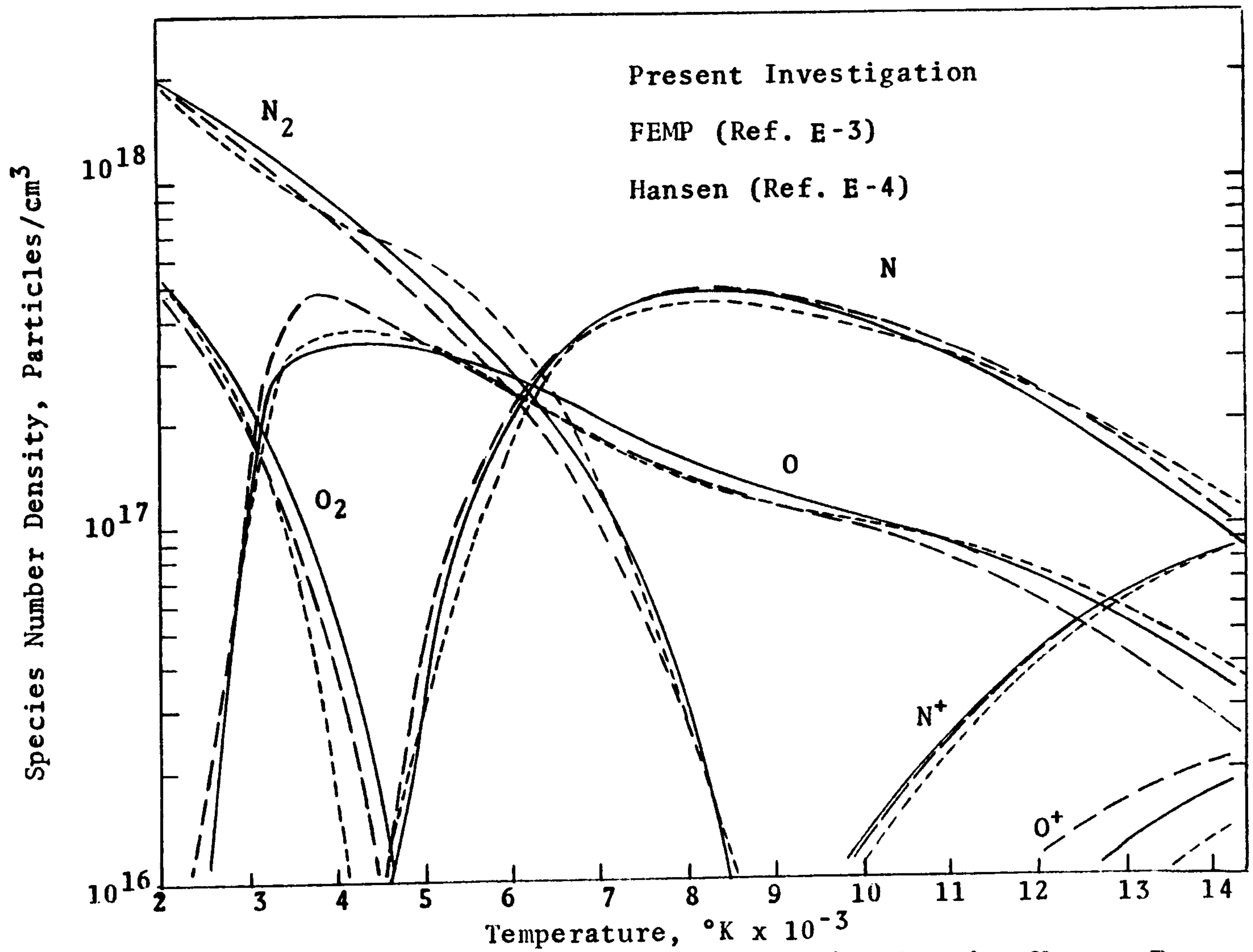

Figure E-1. Comparison of Specie Number Density Versus Temperature Using Several Methods (P=1.0 atm).

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APPENDIX F

COMPUTER PROGRAM FOR A VISCOUS COUPLED STAGNATION LINE HEATING ANALYSIS

The program (SLAB) described in this appendix consists of a numerical solution of the viscous thin shock layer equations presented in Chapter III. A general description of the overall logic and the details of the numerical solutions are given in Chapter V. The program represents the efforts of many individuals over a considerable amount of time. Several of the major subroutines are modifications of previously developed programs dating back as far as 1954. The overall analysis is a modification of a program (VISRAD) primarily developed by Engel (Ref. 5.6). Specifically, the modifications include a solution of the elemental continuity equations with binary diffusion and the addition of a general properties package for the prediction of ablation product transport and thermodynamic properties. A brief description of each of the subprograms included in this code is presented in Table F-1. In the following section, a detailed input guide is given. A complete listing will then follow which includes a sample data package and the corresponding final solution.

Input Guide

The following chart shows the format of the card input.

Card	Variables	Format
1	TITLE	18A4
2	KEEP, NETA, IRAD, ITYPE, MAXM, MAXE, MAXD, LT, IPHI, FPRCT, TPRCT, IDEBUG	9I5, 2E12.0, 2X, I1
3	UINF, RINF, R, TWK, HTØTAL, RVW	5E12.0
4	DELTA, DTIL, RZB, RE, PDTIL	5E12.0
5	T(I)	6E12.0
6A	RHØ(I)	6E12.0
6B	RM(I)	6E12.0
7	DEPS	E12.0
8	ETA(I)	6E12.0
9	NDBUG, TOL	I5, 5X, E10.4
10	CWALL(J)	5E15.8

The meaning of these program variables are as follows:

Variable	Description
TITLE	Title for identification of the problem.
KEEP	Indicator to determine if the temperature profile from the previous case is to be kept as a guess for the current case. KEEP = 0 Temperature not kept KEEP = 1 Temperature kept
NETA	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.
IRAD	A variable used to specify the type of solution. IRAD = 1 Convective solution only = 2 Uncoupled radiation solution = 3 Coupled radiation solution
ITYPE	A variable used to specify the type of radiation model to be used. ITYPE = 0 Line and continuum radiation model = 1 Emission radiation model
MAXM	Maximum number of iterations allowed in the internal momentum loop. If MAXM = 0, it is internally set = 15.
MAXE	Maximum number of iterations allowed in the energy equation and in the overall momentum-energy loop. If MAXE = 0, it is internally set = 15.
MAXD	Maximum number of iterations allowed in the external momentum loop. If MAXD = 0, it is internally set = 15.

Variable	Description
LT	Indicator to determine if a temperature guess and if ρ and $\rho\mu$ guesses are to be read in. LT = 0 Cards 5 and 6 are not read. = 1 Card 5 but not care 6 is read. = 2 Cards 5 and 6 are read.
IPHI	Indicator to determine if the shock curvature is to be input. IPHI = 0 d /d = 0 is internally set. = 1 Card 7 is required for input.
FPRCT	Convergence tolerance for each point in the f' profile. If FPRCT = 0.0 it is internally set = .005.
TPRCT	Convergence tolerance for each point in the T profile. If TPRCT = 0.0 it is internally set = .005.
IDEBUG	A switch to allow intermediate printout to be obtained at each iteration IDEBUG = 0 No print. = 1 Print is given.
UNIF	The freestream flight velocity (U_∞) in feet/sec.
RINF	The freestream density (ρ_∞) in slugs/ft^3.
R	Principal body radius in feet.
TWK	Wall temperature in degrees Kelvin.
HTOTAL	Total freestream enthalpy in ft^2/sec^2. If HTOTAL = 0.0, it is set to $U_\infty^2/2$. (Freestream static enthalpy is assumed negligible).
RVW	Mass injection rate $(\rho v)_W/(\rho U)_\infty$.
DELTA	An initial guess for the shock standoff distance δ/R. If DELTA = 0.0, a guess is supplied by program.

Variable	Description
DTIL	A guess for the transformed standoff distance $\tilde{\delta}/R$. The program will also supply this value if DTIL = 0.0.
RZB	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.
RE	The Reynolds number for the problem, $Re_s = U_\infty R \rho_\delta / \mu_\delta$. This quantity is determined by the program if RE is input as 0.0.
PDTIL	Convergence tolerance placed on $\tilde{\delta}$ for total solution convergence. If PDTIL = 0.0, it is internally set = .001.
T(I),I=1,NETA	An initial guess for the dimensionless shock layer temperature profile (T/T_δ). If LT > 0, this profile is supplied by the user.
RHØ(I),I=1, NETA	An initial guess for the dimensionless shock layer density profile (ρ/ρ_δ). If LT = 2, this profile is supplied by the user.
RM(I),I=1, NETA	An initial guess for the dimensionless shock layer $\rho\mu$ profile $(\rho\mu/\rho_\delta \mu_\delta)$. If LT = 2, this profile is supplied by the user.
DEPS	The stagnation line shock curvature $(d\varepsilon/d\xi)$. If IPHI = 0 then $d\varepsilon/d\xi$ = 0.0 is internally set. If IPHI = 1, card 7 is read and $d\varepsilon/d$ is supplied by the user.
ETA(I),I=1, NETA	The grid shock layer points at which the solution profiles are computed. If NETA = 0, $\Delta\eta$ is set to 0.02 and ETA(I) is computed by the program.
NDBUG	Debug option to output intermediate print from chemical equilibrium calculation. NDBUG = 0 No output. NDBUG = 1 Output given.

Variable	Description
TOL	Convergence criteria for CHEMEQ. If TOL is input as 0.0, the code will set to 0.001.
CWALL(J), J=1,NSP	Wall mass fractions (NSP = 20) species included in order are,

J = 1 = O_2	6 = N^+	11 = CO	16 = C_3H
2 = N_2	7 = E^-	12 = C_3	17 = C_4H
3 = O	8 = C	13 = CN	18 = HCN
4 = N	9 = H	14 = C_2H	19 = C_2
5 = O^+	10 = H_2	15 = C_2H_2	20 = C^+

TABLE F-1

DESCRIPTION OF SLAB SUBPROGRAMS

Subprogram	Description	Additional Subprograms Required
MAIN	Driver program	INPUT, INIT, MOMTM, ERROR, ENERGY, OUTPUT and MULTI
INPUT	Reads in all necessary data and prints out key parameters	none
INIT	Initialization program: Performs shock calculation to determine shock temperature (TD), density ratio (RZB), velocity (VD), and pressure (PD). Estimates shock standoff distance x (DELTA, DTIL). Converts wall and shock compositions to elemental basis. Sets up elemental diffusion coefficient profile.	GAS
MOMTM	Numerical solution to momentum equation as described in Chapter V.	TRID

TABLE F-1 (continued)

Subprogram	Description	Additional Sub-programs Required
ENERGY	Numerical solution of energy equation as described in Chapter V. Serves as driver program for subroutines required for species solution (ELEMNT, CHEMEQ, and PROPRT).	GAS, ELEMNT, CHEMEQ, PROPRT, ELPROF, STPSZE, and TRID
ELEMNT	Numerical solution of elemental continuity equations as described in Chapter V.	FGH, FGHZ, TRID
CHEMEQ	Free energy minimization program for determining equilibrium species compositions. An extensive modification of a program reported by Stroud and Brinkley (Ref. F-1). For further details refer to Appendix E.	ALTERY, THERMO, and MATINV
ALTERY	Adjusts assumed compositions such that desired elemental ratios are obtained. An auxiliary subprogram for CHEMEQ.	none
THERMO	Computes the free energy of the species. Auxiliary program for CHEMEQ.	none

TABLE F-1 (continued)

Subprogram	Description	Additional Sub-programs Required
PROPRT	Calculation of thermodynamic and transport properties by methods described in Chapter IV.	none
GAS	Thermodynamic and transport properties of air, Hansen (Ref. F-2).	none
EFLUX	Correlation developed by Engel (Ref. F-3) for estimation of air radiation properties emission only.	none
LRAD	Driver program for radiation calculation.	TRANS
TRANS	Coupled line and continuum radiation calculation. A modification by Engel (Ref. F-4) of an analysis developed by Wilson (Ref. F-5).	SND, ZHV, BUGPR
SND	Converts mass fractions to number densities. Auxiliary program for TRANS.	none
STPSZE	Adjusts stepsize distribution based on temperature profile.	none

TABLE F-1 (continued)

Subprogram	Description	Additional Subprogram Required
MATINV	Matrix inversion and solution to simultaneous linear equations (Ref. F-1).	none
FGH, FGH2	Three point difference formulas for first and second derivatives (Eqs. 5.15-5.20).	none
TRID	Solution to simultaneous linear equations with tri-diagonal coefficient matrix.	none
QUAD	Trapezoidal rule integration program.	none
OUTPUT	Prints out intermediate and final solutions (See Table F-3). Also punches intermediate and converged solutions for use in restarting.	TRANS, EFLUX, TRANSZ
ERROR	Prints out a diagnostic message when energy and/or momentum solutions fail to converge.	none
ELPROF	Prints out intermediate solutions to elemental continuity equations.	none

TABLE F-1 (continued)

Subprogram	Description	Additional Subprogram Required
MULTI	Punches out data package for multicomponent diffusion analysis (SLAM).	none
BLOCK DATA	Data package containing the following information: Optional initial guesses for ρ, $\rho\mu$, and T profiles; Alphameric labels for species identification; molecular weights; coefficients for individual viscosity and thermal conductivity curve fits (Discussed in Chapter IV); polynomial coefficients for thermodynamic properties (Chapter IV); atomic weights of the elements; and the matrix of elemental ratios (A_{ij}'s, See Appendix A) for the species considered.	none

REFERENCES

F-1. Stroud, C. W. and K. L. Brinkley, "Chemical Equilibrium of Ablation Materials Including Condensed Species," NASA TN D-5391 (August, 1969).

F-2. Hansen, C. F., "Approximations for the Thermodynamic Properties of High Temperature Air," NASA TR R-50, 1959.

F-3. Engel, C. D., and L. W. Spradley, Radiation Absorption Effects on Heating Loads Encountered During Hyperbolic Entry, JSR, Vol. 6, No. 6, pp. 764-766, June 1969.

F-4. Engel, C. D. "Ablation and Radiation Coupled Viscous Hypersonic Shock Layers," Ph.D. Dissertation, Louisiana State University, Baton Rouge, Louisiana (1971).

F-5. Wilson, K. H., "Stagnation Point Analysis of Coupled Viscous-Radiating Flow with Massive Blowing," NASA CR-1548 (June, 1970).

```
C     ** SLAB - STAGNATION LINE HEATING  ANALYSIS (BINARY DIFFUSION)
C        FOR A VISCOUS HYPERSONIC SHOCK LAYER WITH RADIATIVE HEAT
C        TRANSFER.      C. D. ENGEL AND D. D. ESCH    JULY 1971
C
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,IDEBUG,MCONV,ECONV,DCONV,LT,IAB
      LOGICAL MCONV,ECONV,DCONV
C
C
C
C     **          D R I V E R    P R O G R A M           **
C
C
    1 CONTINUE
C
C     **  READ AND PRINT ALL INPUT DATA  **
C
      CALL INPUT
C
C     **  COMPUTE NECESSARY INITIAL QUANTITIES  **
C
      CALL INIT
      IEM = 0
C
C
C     **  SOLVE MOMENTUM EQUATION  **
C
 1000 CONTINUE
      IEM = IEM+1
C
      CALL MOMTM
C
C     **  CHECK FOR CONVERGENCE OF MOMENTUM ITERATION  **
C
      IF ( MCONV ) GO TO 1500
C
```

```
C
C     **  ERROR EXIT IF MOMENTUM ITERATION DOES NOT CONVERGE  **
C
      CALL ERROR ( 1 )
C
 1500 CONTINUE
C
C     **  SOLVE ENERGY EQUATION  **
C
      CALL ENERGY
C     **  INTERMEDIATE PRINTOUT OF TEMPERATURE ITERATION  **
C
      IF( IDEBUG.GT. 0 )                   CALL OUTPUT(2)
C
C     **  CHECK FOR CONVERGENCE OF TEMPERATURE ITERATION  **
C
C
      IF( ECONV ) GO TO 2500
C
C     **  ERROR EXIT IF TEMPERATURE ITERATION DOES NOT CONVERGE  **
C
      CALL ERROR ( 2 )
C
 2500 CONTINUE
C
C     **  CHECK SIMULTANEOUS MOMENTUM AND ENERGY CONVERGENCE  **
C
      IF(IEM.EQ.2.OR.IEM.EQ.4)GOTO1000
      IF(IEM.GT.MAXD) GO TO 3000
      IF(.NOT.MCONV) GO TO 1000
      IF(.NOT.FCONV) GO TO 1000
      IF(.NOT.DCONV) GO TO 1000
C     **  PRINT ALL OUTPUT  **
C
      CALL OUTPUT ( 1 )
      CALL MULTI
```

```
C
C     **  CONVERGED , GO BACK TO RUN ANOTHER CASE  **
C
      GO TO 1
C
 3000 CONTINUE
C
C     **  MOMENTUM AND ENERGY DID NOT CONVERGE SIMULTANEOUSLY  **
C
      CALL ERROR(3)
      CALL OUTPUT (3)
      GO TO 1
      END
```

```
      SUBROUTINE INPUT
C
C
C     **  ROUTINE TO READ AND PRINT ALL INPUT DATA  **
C
C
      COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,IDEBUG,MCONV,ECONV,DCONV,LT,IAB
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(50),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 /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON/WALL/RVW,PRW,TWOLD,FLUX(20),CWALL(20),ECWALL(5)
      COMMON /YL/ETA(60),YOND(60)
C
C
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X         AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/EQ2/AA(20,5),ICODE(20)
      COMMON/EQ3/IA(20,5)
      COMMON/ID/SP(20),EL(5)
      COMMON/WT/SMW(20),AWT(5)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON/SP1/SS,TOL,NDBUG
C
      REAL  MU,MUDZ
      LOGICAL MCONV,ECONV,DCONV
      DIMENSION TITLE(18)
      DATA END /'END '/
      IF ( TITLE ( 1 ) .EQ. END ) STOP
C
C
C
C     **  INPUT FORMATS  **
```

```
C
 100  FORMAT (18A4)
 101  FORMAT (9I5,2E12.0,2X,I1)
 102  FORMAT ( 6E12.0 )
 103  FORMAT(A4,6X, E10.4,20X,5F5.0,F10.5)
 104  FORMAT(7E10.4)
 105  FORMAT(A4,E16.8)
 106  FORMAT(6E10.4,I3)
 107  FORMAT(I5,  5X,E10.4,I5)
 108  FORMAT(5E15.8)
C
C      **  OUTPUT FORMATS  **
C
 200  FORMAT ( 1H1 , 18A4 //// )
 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   )
 204  FORMAT ( 9H0UINF   = 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 //)
C
 206  FORMAT ( 20H0INITIAL T PROFILE  / ( 1H , 12F10.5 )     )
 207  FORMAT ( 20H0INITIAL RHO PROFILE/ ( 1H , 12F10.5 )     )
 208  FORMAT ( 20H0INITIAL RM  PROFILE/ ( 1H , 12F10.5 )     )
```

```
  210  FORMAT(32H * CONVECTIVE 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
  216  FORMAT (16H SPECIES INPUTS                                       INPU 790
      1        /16H NO. ELEMENTS = I5                                   INPU 800
      2        /25X,5(I5,2X,A4)      )                                  INPU 810
  218  FORMAT (16H NO. SPECIES  = I5)                                   INPU 820
  220  FORMAT (25X,5(I5,2X,A4))                                         INPU 830
  222  FORMAT (16H NO. SOLIDS   = I5)                                   INPU 840
C                                                                       INPU 850
C CARD 1 -------------------------------------------------------------- INPU 860
       READ (5,100) TITLE                                               INPU 870
       IF ( TITLE ( 1 ) .EQ. END ) STOP                                 INPU 875
       WRITE ( 6,200 ) TITLE                                            INPU 880
C                                                                       INPU 890
C                                                                       INPU 900
C      **  INPUT OPTION PARAMETERS  **                                  INPU 910
C                                                                       INPU 920
C      **  IRAD = 1  NO RADIATION CALCULATED                            INPU 930
C          IRAD = 2  UNCOUPLED SOLUTION                                 INPU 940
C          IRAD = 3  COUPLED SOLUTION  **                               INPU 950
C      **  ITYPE=0 SPECTRAL MODEL WITH LINES                            INPU 960
C          ITYPE=1 EMISSION MODEL                                       INPU 970
C                                                                       INPU 980
       KETA = NETA                                                      INPU 990
C CARD 2 -------------------------------------------------------------- INPU1000
       READ (5,101)KEEP,NETA,IRAD,ITYPE,MAXM,MAXE,MAXD,LT,IPHI,         INPU1010
      1           FPRCT,TPRCT,IDEBUG                                    INPU1020
       META = NETA                                                      INPU1030
       IF(KETA .EQ. 0) KEEP = 0                                         INPU1040
       IF(KEEP. GT. 0) NETA = KETA                                      INPU1050
C                                                                       INPU1060
       DDAMP = 0.5                                                      INPU1070
       TDAMP = 0.6                                                      INPU1080
```

```
      IF(MAXM .EQ. 0) MAXM=15                                           INPU1090
      IF(MAXE.EQ. 0) MAXE=20                                            INPU1100
      IF(MAXD.EQ. 0) MAXD=15                                            INPU1110
      IF(FPRCT.EQ. 0.0) FPRCT=.005                                      INPU1120
      IF(TPRCT .EQ. 0.0) TPRCT=0.005                                    INPU1130
      IF ( NETA .EQ. 0 ) NETA = 51                                      INPU1140
      IF (IRAD.EQ.0) IRAD =1                                            INPU1150
C                                                                       INPU1160
      WRITE ( 6,201 )                                                   INPU1170
      WRITE (6,202)KEEP,NETA,MAXM,MAXE,MAXD,FPRCT,TPRCT,LT,IDEBUG       INPU1180
     1                ,IPHI                                             INPU1190
C                                                                       INPU1200
C     **  FREE-STREAM FLIGHT CONDITIONS  **                             INPU1210
C CARD 3 -------------------------------------------------------------- INPU1220
      READ(5,102) U INF,R INF,R,TWK,HTOTAL,RVW                          INPU1230
      UINF2=UINF**2                                                     INPU1240
      IF(KEEP.GT. 0) TWOLD = T(1)                                       INPU1250
      T(1)=TWK                                                          INPU1260
C                                                                       INPU1270
      IF(HTOTAL .EQ. 0.0) HTOTAL=UINF2/2.0                              INPU1280
C                                                                       INPU1290
C     **  INITIAL SHOCK QUANTITY ESTIMATES  **                          INPU1300
C CARD 4 -------------------------------------------------------------- INPU1310
      READ(5,102) DELTA,DTIL,RZB,RE,PDTIL                               INPU1320
      IF(PDTIL.EQ.0.0) PDTIL = .001                                     INPU1330
      WRITE(6,204) U INF,R INF,R,TWK,HTOTAL,RVW,PDTIL                   INPU1340
      IF (IRAD.EQ.1) WRITE (6,210)                                      INPU1350
      IF (IRAD.EQ.2) WRITE (6,211)                                      INPU1360
      IF (IRAD.EQ.3) WRITE (6,212)                                      INPU1370
      IF(IRAD.EQ.1) GO TO 300                                           INPU1380
      IF( ITYPE.EQ.0) WRITE(6,213)                                      INPU1390
      IF( ITYPE.EQ.1) WRITE(6,214)                                      INPU1400
  300 CONTINUE                                                          INPU1410
C                                                                       INPU1420
C     **   INPUT INITIAL TEMPERATURE PROFILE   **                       INPU1430
C CARD 5 -------------------------------------------------------------- INPU1440
```

```
      IF(LT .EQ. 0) GO TO 2800                                          INPU1450
      READ ( 5,102 ) ( T ( I ) , I = 1 , NETA )                         INPU1460
      WRITE ( 6,206 ) ( T ( I ) , I = 1 , NETA )                        INPU1470
      T(1) =TWK                                                         INPU1480
 2800 CONTINUE                                                          INPU1490
C     ** INPUT RHO AND (RHO)(MU) PROFILES  **                           INPU1500
C CARD 6 -------------------------------------------------------------- INPU1510
      IF(LT.LT.2) GO TO 2900                                            INPU1520
      READ(5,102) (RHO(I),I=1,NETA)                                     INPU1530
      READ(5,102) (RM (I),I=1,NETA)                                     INPU1540
      WRITE(6,207)(RHO(I),I=1,NETA)                                     INPU1550
      WRITE(6,208)(RM (I),I=1,NETA)                                     INPU1560
 2900 CONTINUE                                                          INPU1570
C                                                                       INPU1580
C     **  SHOCK SHAPE (DEPS/DXI)  **                                    INPU1590
C                                                                       INPU1600
      IF (IPHI .NE. 0 ) GO TO 2550                                      INPU1610
      DEPS = 0.0                                                        INPU1620
      GO TO 2570                                                        INPU1630
 2550 CONTINUE                                                          INPU1640
C CARD 7 -------------------------------------------------------------- INPU1650
      READ(5,102)  DEPS                                                 INPU1660
 2570 CONTINUE                                                          INPU1670
      DPHI = 1. -DEPS                                                   INPU1680
      WRITE(6,217)  DEPS                                                INPU1690
 217  FORMAT(9HODEPS/DXI  /(1H ,12F10.5) )                              INPU1700
C                                                                       INPU1710
C                                                                       INPU1720
      IF ( META .GT. 0 ) GO TO 1000                                     INPU1730
      IF(KEEP .GT. 0) GO TO 1500                                        INPU1740
C                                                                       INPU1750
C     **  FIXED GRID SIZE ON ETA  **                                    INPU1760
C                                                                       INPU1770
      DETA = 0.02                                                       INPU1780
      ETA ( 1 ) = 0.0                                                   INPU1790
      DO 500 I = 2 , 51                                                 INPU1800
```

```
      ETA ( I ) = ETA ( I-1 ) + DETA                                    INPU1810
  500 CONTINUE                                                          INPU1820
C                                                                       INPU1830
      GO TO 1500                                                        INPU1840
C                                                                       INPU1850
 1000 CONTINUE                                                          INPU1860
C                                                                       INPU1870
C     **  INPUT ETA POINTS  **                                          INPU1880
C CARD 8 ---------------------------------------------------------------INPU1890
      READ ( 5,102 ) ( ETA ( I ) , I = 1 , NETA )                       INPU1900
C                                                                       INPU1910
 1500 CONTINUE                                                          INPU1920
C                                                                       INPU1930
C-----READ SPECIES PARAMETER CARDS......                                INPU1940
C CARD 9 ---------------------------------------------------------------INPU1950
      READ 107,NDBUG,TOL                                                INPU1960
C                                                                       INPU1970
      IAB = 1                                                           INPU1980
      IF(TOL.LE.0.0) TOL = .001                                         INPU1990
C     NDBUG=OPTIONAL OUTPUT VARIABLE                                    INPU2000
C     NC = NUMBER OF GASEOUS COMPONENTS                                 INPU2010
C CARD 10 --------------------------------------------------------------INPU2020
      READ 108,(CWALL(I),I=1,NSP)                                       INPU2030
      WRITE(6,216) NE,(I,EL(I),I=1,NE)                                  INPU2040
      WRITE(6,218) NSP                                                  INPU2050
      JJ = 1                                                            INPU2060
      KK = JJ+4                                                         INPU2070
   30 WRITE(6,220) (I,SP(I),I=JJ,KK)                                    INPU2080
      IF(KK+5.GT.NSP) GO TO 35                                          INPU2090
      JJ = JJ+5                                                         INPU2100
      KK = JJ +4                                                        INPU2110
      GO TO 30                                                          INPU2120
   35 KD = NSP -KK                                                      INPU2130
      IF(KD.LE.0) GO TO 45                                              INPU2140
      KK = KK +KD                                                       INPU2150
      JJ = JJ +5                                                        INPU2160
```

```
40    GO TO 30
45    CONTINUE
      WRITE(6,222) NNS
      PRINT 305
305   FORMAT(/' SPECIES'/' NAME',9X,'SMW',                          2X,
     1'WALL MASS FRACTION'/)
      DO10I=1,NSP
10    PRINT302,SP(I),SMW(I),CWALL(I)
302   FORMAT(1X,A4,1F13.3,E12.4)
      IF(NDBUG.EQ.0)GOTO9999
      PRINT309
309   FORMAT(//,' SPECIES',35X,'THERMO-CONSTANTS A-G',29X,'RANGE')
      DO11I=1,NSP
      PRINT303,SP(I),AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)
11    PRINT304,       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)
9999  CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE INIT
C
C
C     **  ROUTINE TO COMPUTE NECESSARY INITIAL QUANTITIES
C
C
      COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON/EQ2/AA(20,5),ICODE(20)
      COMMON/EQ3/IA(20,5)
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON/GUESS/TG1(60),TG2(60)
      COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,IDEBUG,MCONV,ECONV,DCONV,LT,IAB
      COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON/NUMBER/NSP,NNS,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/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/RVW,PRW,TWOLD,FLUX(20),CWALL(20),ECWALL(5)
      COMMON/WT/SMW(20),AWT(5)
      COMMON /YL/ETA(60),YOND(60)
      COMMON /DIF/ D(5,60)
      REAL  MU,MUDZ
C
      LOGICAL MCONV,ECONV,DCONV
C
      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
C     **  DETERMINE DENSITY RATIO , REYNOLDS NUMBER
C         FROM INPUTS OR RANKINE HUGONIOT EQS.   **
C
C GUESSED VALUES
      TD = 12000. + .5E-5*(HTOTAL -6.5E+8)
      RZ3=.06
C
      T(NETA) = 1.0
      HNF = 2.*778.28*32.172/UINF2
 998  CONTINUE
      PD = (1. -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)
      PI(NETA) = PD
      CALL GAS(NETA)
      RZB1=RINF/(RDZ*RHO(NETA) )
      TEST =ABS((RZB-RZB1)/RZB)
      IF(TEST .LT. 0.005) GO TO 999
      RZB=.5*(RZB+RZB1)
      GO TO 998
 999  CONTINUE
      RE = PDZ*UINF*R*32.174 / MUDZ
C
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,12HREYNOLDS NO.  /2E15.6)
      WRITE(6,201) DELTA,DTIL
 201  FORMAT(6HODFLTA,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(1)
      T(1) = T(1)/TD
C
C     **  STAGNATION POINT LIMIT QUANTITIES  **
C
      DUD = DPHI + RZB*(1.-DPHI)
C NONDIMENSIONALIZING FACTORS
      AKNF = 1.8*778.28*TD       *RZB/(R*RINF*UINF*UINF2)
      CPNF = 1.8*778.28*32.172*TD *2.   /UINF2
C
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
      DO 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.0.0)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
    7 CONTINUE
      TWG2 = .3325
C BLOWING T PROFILE
      DO8K = 2,NETA
      TP = TG2(K) +(T(1)- TWG2)
      T(K) = TP -(T(1)- TWG2) * ETA(K)
    8 CONTINUE
      GO TO 11
    9 CONTINUE
      DO 10 K=2,NETA
      TP = T(K) +T(1) -TWOLD
      T(K) = TP -(T(1)-TWOLD)*ETA(K)
      WRITE(6,100) T(K),ETA(K)
 10   CONTINUE
 11   CONTINUE
C
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)
      AK(I) = AK(NETA)
      V(I) = VD
      F(I) = FD
      FC(I)=FD
      DO 810 J=1,NSP
```

```
      C(J,I) = C(J,NETA)
      HS(J,I)=1.0
  810 CONTINUE
 1000 CONTINUE
C
      DO221I=1,NSP
      C(I,1) = CWALL(I)
  221 CONTINUE
C-----CALCULATE AMW(N)
C
      WAMW = 0.0
      DO 25 J=1,NSP
   25 WAMW = WAMW +CWALL(J)/SMW(J)
      WAMW = 1./WAMW
   26 AMW(1)= WAMW
C
C-----FLOAT AA(I,J) MATRIX....
C
      DO30I=1,NSP
      DO30J=1,NE
   30 AA(I,J)=IA(I,J)
C
      IF(ITYPE.EQ.C)CALL RADIN
C
C-----CONVERT WALL AND SHOCK COMPOSITIONS TO AN ELEMENTAL BASIS.....
C
      DO331J=1,NE
      EC(J,1)=0.0
      EC(J,NETA)=0.0
      DO33I=1,NSP
      FAC=AA(I,J)*AWT(J)/SMW(I)
      EC(J,1)=EC(J,1) + FAC*C(I,1)
   33 EC(J,NETA)=EC(J,NETA) + FAC*C(I,NETA)
  331 ECWALL(J)=EC(J,1)
C
      DO34N=NETA,60
```

```
      DO34J=1,NE                                                        INIT1810
   34 EC(J,N)=EC(J,NETA)                                                INIT1820
C                                                                       INIT1830
C-----INITIALIZE ELEMENTAL DIFFUSION COEFFICIENTS....                    INIT1840
C                                                                       INIT1850
      DO35N=1,NETA                                                      INIT1860
      TT=T(N)*TD                                                        INIT1870
      DO35J=1,NE                                                        INIT1880
   35 D(J,N)=0.8128E-07*(TT**1.659)/(PI(N)*R*JINF)                      INIT1890
C                                                                       INIT1900
C                                                                       INIT1910
      DTILS = .01                                                       INIT1920
      IF(IDEBUG .EQ. 0) RETURN                                          INIT1930
      WRITE(6,4000) VD,DUD,PD                                           INIT1940
      WRITE(6,4000) DELTA,DTIL,RZB,RE                                   INIT1950
 4000 FORMAT(1H0,6E15.6)                                                INIT1960
  203 FORMAT(6E12.0)                                                    INIT1970
  100 FORMAT(1X,9E14.6)                                                 INIT1980
      RETURN                                                            INIT1990
      END                                                               INIT2000
```

```
      SUBROUTINE MOMTM
C
C -----THIS SUBROUTINE SOLVES THE MOMENTUM EQUATION AS A
C       SECOND ORDER EQUATION AND A FIRST ORDER EQUATION -----
C
      COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /FRSTRM/ U INF, 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/PROP1/PI(60),RHO(60), T(60),AMW(50),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,ITYPE
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON/VECTOR/ CA(60),CB(60),CC(60),B(60)
      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)
      LOGICAL MCONV,ECONV,DCONV
C
C----- INITIALIZED QUANTITIES -----
C
      MCONV = .FALSE.
      ITM = 1
      N = NETA -2
      L = NETA-1
      AA3 = RZB*(1.-RZB)*DPHI**2/DUD
      IF(IEM.GT.3) DTIL=.5*(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*DUD
      DTIL2 = DTIL*DTIL
      FD = RZB/(2.*DUD*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)
      DETN=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*( AA3/(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,CB,CC
      CA(II) =(2.-A1*DETN)/D3
      CB(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
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-1)+B(K-2))*(ETA(K) -ETA(K-1))/2.
   30 FC(K) = SUM
C
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 65I=1,N
   65 Z(I)=B(I)
      IF(ITER.GE.MAXM ) GO TO 90
      GO TO 15
   90 CONTINUE
C
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.PDTIL) GO TO 150
      DTIL = DTIL +DDAMP*(DTILC-DTIL)
      GO TO 14
  150 CONTINUE
      DTIL = DTIL+ DDAMP*(DTILC -DTIL)
      MCONV = .TRUE.
C
```

```
C CHECK MOMENTUM-ENERGY CONVERGENCE                                     MOMT1090
      PRCT = ABS((DTIL-DTILS)/DTILS)                                    MOMT1100
      IF(PRCT.LE.PDTIL) DCONV = .TRUE.                                  MOMT1110
  160 CONTINUE                                                          MOMT1120
C                                                                       MOMT1130
      DO 170 K=1,NETA                                                   MOMT1140
  170 V(K) = -FC(K)*DTIL*2./RHO(K)                                      MOMT1150
      DTILS2 = DTILS                                                    MOMT1160
C DEBUG OUTPUT                                                          MOMT1170
      IF(IDEBUG.EQ. 0) RETURN                                           MOMT1180
      WRITE(6,102) ITER,ITM                                             MOMT1190
      WRITE(6,100) DTIL,DTILC                                           MOMT1200
      DO 120 K=1,NETA                                                   MOMT1210
      VS=-FC(K)*DTIL*UINF*2./RHO(K)                                     MOMT1220
      WRITE(6,100) ETA(K),F(K),FC(K),  RHO(K),RM(K),VS ,V(K)            MOMT1230
  120 CONTINUE                                                          MOMT1240
      DO 121 I=1,N                                                      MOMT1250
      U=B(I)*DTIL                                                       MOMT1260
      WRITE(6,100) ETA(I+1),Z(I),B(I),U                                 MOMT1270
  121 CONTINUE                                                          MOMT1280
  100 FORMAT(1X,9E14.6)                                                 MOMT1290
  102 FORMAT(10X,2I3/)                                                  MOMT1300
      RETURN                                                            MOMT1310
      END                                                               MOMT1320
```

```
      SUBROUTINE ENERGY
C
C-----THIS SUBROUTINE SOLVES THE ENERGY EQUATION
C     IN A GLOBALLY IMPLICIT MANNER---------
C
      COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /FRSTRM/ U INF, 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,NNS,NE,NC
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(50),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,ITYPE
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON/SP2/BR,S(20),CSHOCK(5)
      COMMON/VECTOR/ CA(60),CB(60),CC(60),B(60)
      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 /OLD/ TOLD(60),EOLD(60),RHOS(60)
      DIMENSION          RHOLD(60)
      REAL  MU,MUDZ
      LOGICAL MCONV,ECONV,DCONV
C
C-----INITIALIZED QUANTITIES-----
C
      ECONV = .FALSE.
      DTILN = DTIL
      IF(IEM.GE. 2) DTIL= DTILN+.45*(DTILS -DTILN)
      DTILS = DTILN
      NF=NETA
      N=NETA-2
      ITER = 0
      EPRCT=.5
```

```
      DO 3 I=1,NETA                                                    ENER 370
      EOLD(I)=E(I)                                                     ENER 380
      RHOS(I)=RHO(I)                                                   ENER 390
    3 TOLD(I) = T(I)                                                   ENER 400
C                                                                      ENER 410
      IF(ITYPE.NE.0.OR.IRAD.NE.3)GOTO7                                 ENER 430
      CALL GAS(1)                                                      ENER 440
      IF(RVW.LE.0.0)NSP=7                                              ENER 460
      CALL ELEMNT                                                      ENER 470
      CALL CHEMEQ(1,NF)                                                ENER 480
      CALL PROPRT(NSP,1,NF)                                            ENER 490
C                                                                      ENER 500
    7 CONTINUE                                                         ENER 510
      IF(IRAD.EQ.3.AND .ITYPE.EQ.1) CALL EFLUX                         ENER 520
      IF(IRAD.EQ.3.AND.ITYPE.EQ.0)CALL LRAD                            ENER 530
C                                                                      ENER 540
      IF(IEM.EQ.1)GOTO9                                                ENER 550
      DO8I=1,NETA                                                      ENER 560
    8 E(I)=EPRCT*E(I) + (1.-EPRCT)*EOLD(I)                             ENER 570
    9 CONTINUE                                                         ENER 580
C                                                                      ENER 590
   10 CONTINUE                                                         ENER 600
C                                                                      ENER 610
      NS = NSP                                                         ENER 620
      CALL GAS(1)                                                      ENER 630
C                                                                      ENER 660
      CALL ELEMNT                                                      ENER 670
      CALL CHEMEQ(1,NETA)                                              ENER 680
      CALL PROPRT(NSP,1,NETA)                                          ENER 690
C                                                                      ENER 710
   11 CONTINUE                                                         ENER 720
C                                                                      ENER 730
C-----T''+A1*T'=A2                                                     ENER 740
C     COMPUTE A1 AND A2                                                ENER 750
C                                                                      ENER 760
      II = 1                                                           ENER 770
```

```
      DO 20 I=1,N
      DET=ETA(I+1)-ETA(I)
      DETN=ETA(I+2)-ETA(I+1)
      C1= DET/(DETN*(DETN+DET))
      C2=(DETN-DET)/(DETN*DET)
      C3=DETN/(DET*(DETN+DET))
      COEF=DTIL/(2.*RHO(I+1)*AK(I+1))
C
C-----A1-------
C
      TARM1=RHO(I+1)*V(I+1)*CP(I+1)
      TARM2=0.0
      TARM3=C1*RHO(I+2)*AK(I+2)+C2*RHO(I+1)*AK(I+1)
     1    -C3*RHO(I)*AK(I)
      A1=-COEF*(TARM1+TARM2-TARM3)
C
C-----A2------
C
      TERM1=0.0
      IF(I.GE.NF) NS= 7
      IF(IEM.LT.IAB) NS=7
      DO 16 J=1,NS
      TERM1=TERM1+HS(J,I+1)*(C1*C(J,I+2)+C2*C(J,I+1)
     1                     -C3*C(J,I))
   16 CONTINUE
      TERM1 = 0.0
      TERM2=2.*V(I+1)*(C1*V(I+2)+C2*V(I+1)-C3*V(I))
      TERM3=0.0
      A2=COEF*(RHO(I+1)*V(I+1)*(TERM1+TERM2)
     1        +TERM3+2.*DTIL*E(I+1)/RHO(I+1) )
C
C-----CA*T(N-1)+CB*T(N)+CC*T(N+1)=B
C
      CA(II) = C3*(-A1+2./DETN)
      CB(I) =C2* A1 -2./(DETN*DET)
      CC(I) = C1*(A1+2./DET)
```

```
      IF (I.EQ.1) BC=CA(1)*T(1)
      B(I)=A2-BC
      BC=0.0
      II = I
   20 CONTINUE
      B(N)=A2-CC(N)
C
      CALL TRID (N)
C
C-----CHECK FOR CONVERGENCE
C
      DO 30 I=1,N
      IF(B(I).LT.T(1))GOTO30
      PRCT=ABS((B(I)-T(I+1))/T(I+1))
      IF (PRCT.GT.TPRCT) GO TO 40
   30 CONTINUE
      GO TO 90
   40 ITER=ITER+1
      DO 50 I=1,N
      II=I+1
      T(II) = T(II) +TDAMP*(B(I)-T(II))
      IF(T(II).GT.1.0) T(II) = .99999
      IF(T(II).LT.T(1)) T(II)=1.000001*T(1)
   50 CONTINUE
      IF(ITER.GE.MAXE ) GOTO 90
      GO TO 10
   90 CONTINUE
      IF(ITER.LT.MAXE) ECONV=.TRUE.
C     IF(IEM.EQ.2.OR.IEM.EQ.4) CALL STPSZE
C
      TMCH=.08
      DO 91 I=1,N
      II = I+1
      T(II) = T(II) +.35*(TOLD(II) -T(II))
      PRCT=(T(II)-TOLD(II))/TOLD(II)
      IF(ABS(PRCT).GT.TMCH)T(II)=TOLD(II)+TMCH*PRCT*TOLD(II)/ABS(PRCT)
```

```
 91   CONTINUE
      ITER = 0
 915  ITER = ITER + 1
      IF(ITER.GT.5)GOTO9251
      DO92I=1,NETA
 92   RHOLD(I)=RHO(I)
      CALL ELEMNT
      CALL CHEMEQ(1,NETA)
      CALL PROPRT (NSP,1,NETA)
      DO925I=1,NETA
      ERR=ABS(RHOLD(I)-RHO(I))/RHO(I)
      IF(ERR.GT..01)GOTO0915
 925  CONTINUE
 9251 CONTINUE
C
C-----NEW GUESS FOR DENSITY PROFILE....
C
      IF(IEM.EQ.1)GOTO927
      DO926I=1,NETA
 926  RHO(I)=RHO(I)*.7 + RHOS(I)*.3
 927  CONTINUE
      IF(IDEBUG.GT.0) CALL ELPROF
 93   CONTINUE
      DTIL = DTILN
C DEBUG OUTPUT
      IF(IDEBUG.EQ. 0) RETURN
      WRITE(6,102) ITER
      DO 95 K=1,NETA
      TK = T(K) *TD
      WRITE (6,100) ETA(K),TK,E(K)
  95  CONTINUE
  100 FORMAT(1X,9E14.6)
  102 FORMAT(10X,I3/)
      RETURN
      END
```

```
      SUBROUTINE ELEMNT                                                 ELEM  10
      COMMON/NUMBER/NS,NNS,NE,NC                                        ELEM  20
      COMMON /MCD1/JS(20, 60),JE(5, 60)                                 ELEM  30
      COMMON/PRCP1/PI( 60),RO( 60),TT( 60),AMW( 60),C (20, 60),CC(5, 60)ELEM  40
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM, NETA   ELEM  50
      COMMON /VECTOR/SUB( 60),DIAG( 60),SUP( 60),B( 60)                 ELEM  60
      COMMON /SCE/ NCHECK,ITER                                          ELEM  70
      COMMON/SP1/SS,TOL,NDBUG                                           ELEM  80
      COMMON /DIF/D(5, 60)                                              ELEM  90
      COMMON /YL/ ET( 60),YOND( 60)                                     ELEM 100
      COMMON /VEL/FF( 60),FC( 60),ZZ( 60),VV( 60)                       ELEM 110
      COMMON /DEL/ DELTA,DTIL,DTILS                                     ELEM 120
      COMMON/WALL/RVW,PRW,TWOLD,FLUX(20),CWALL(20),ECWALL(5)            ELEM 130
      DIMENSION TEF(5, 60)                                              ELEM 140
      DIMENSION XM(5)                                                   ELEM 150
      REAL JS, JE                                                       ELEM 160
      NCHECK=0                                                          ELEM 170
      NM1=NETA-1                                                        ELEM 180
      IF(RVW.LE.0.0) GO TO 200                                          ELEM 185
      DO15J=1,NE                                                        ELEM 190
   15 XM(J)=RO(1)*VV(1)*ECWALL(J)                                       ELEM 200
      M=1                                                               ELEM 210
C                                                                       ELEM 220
  150 DO180J=1,NE                                                       ELEM 230
      DIAG(1)= 1.0 + ET(2)*DTIL*VV(1)/(RO(1)*D(J,1))                    ELEM 240
      SUP(1)=-1.0                                                       ELEM 250
      B(1)=DTIL*XM(J)*ET(2)/(RO(1)*RO(1)*D(J,1))                        ELEM 260
  154 DO155K=2,NETA                                                     ELEM 270
      N=M-1+K                                                           ELEM 280
      CALL FGH(N,F1,G1,H1)                                              ELEM 290
      CALL FGH2(N,F2,G2,H2)                                             ELEM 300
      DLNRO=F1*RO(N+1)/RO(N) + G1 + H1*RO(N-1)/RO(N)                    ELEM 310
      DLNDJ=F1*D(J,N+1)/D(J,N) + G1 + H1*D(J,N-1)/D(J,N)                ELEM 320
      PETA=-DTIL*VV(N)/(RO(N)*D(J,N)) + 2.*DLNRO + DLNDJ                ELEM 330
      SUB(K-1)= PETA*H1 + H2                                            ELEM 340
      DIAG(K)= PETA*G1 + G2                                             ELEM 350
```

```
      SUP(K)= PETA*F1 + F2
      B(K)=0.0
      IF(N.GE.(NETA-1))GOTO160
155   CONTINUE
160   B(K)=-SUP(K)*CC(J,NETA)
      CALL TRID(K)
      DO170L=1,K
      COLD=CC(J,M-1+L)
      CC(J,M-1+L)=B(L)
      ERR=ABS(CC(J,M-1+L) -COLD)
      IF(ERR.GE..01)NCHECK=NCHECK+1
170   CONTINUE
180   CONTINUE
      RETURN
 200  CONTINUE
      DO210 J=1,NE
      DO210 N=1,NM1
      CC(J,N)=CC(J,NETA)
 210  CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CHEMEQ( NI,NF)                                             CHEM
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * CHEM
C                                                                         * CHEM
C     THIS SUBPROGRAM IS A REVISION OF A PROGRAM ORIGINALLY REPORTED      * CHEM
C     IN NASA-TN-D-5391 (AUGUST 1969).   THE PROGRAM COMPUTES FOR A       * CHEM
C     PRESSURE ARRAY,PP(N),TEMPERATURE ARRAY,TT(N), AND AN ARRAY          * CHEM
C     OF ELEMENTAL MASS FRACTIONS-CC(I,N), THE EQUILIBRIUM SPECIES        * CHEM
C     MASS FRACTIONS AT EACH POINT-N REPRESENTED BY THE GIVEN ARRAYS.     * CHEM
C     THE EQUILIBRIUM COMPOSITIONS ARE STORED IN THE MATRIX CE(I,N).      * CHEM
C                                                                         * CHEM
C                                     DONALD D. ESCH                      * CHEM
C                                     LOUISIANA STATE UNIVERSITY          * CHEM
C                                     AUGUST 7, 1970                      * CHEM
C                                                                         * CHEM
C                                                                         * CHEM
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * CHEM
C     IN = INITIAL POINT FOR EQUILIBRIUM CALCULATIONS.                    * CHEM
C     NF = FINAL POINT.                                                   * CHEM
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * CHEM
      COMMON/WALL/RVW,PRW,TWOLD,FLUX(20),CWALL(20),ECWALL(5)                CHEM
      COMMON/SP1/SS,TOL,NDBUG                                               CHEM
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),CHEM
     X           AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20) CHEM
      COMMON/EQ2/AA(20,5),ICODE(20)                                         CHEM
      COMMON/THERM1/C(20),FORT(20)                                          CHEM
      COMMON/ID/SP(20),EL(5)                                                CHEM
      COMMON/NUMBER/NS ,NNS,MM,NC                                           CHEM
      COMMON/WT/XMW(20),AWT(5)                                              CHEM
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL                              CHEM
      COMMON /DY/ DYDT(20,60)                                               CHEM
      COMMON/PROP1/PP(60),RO(60),TT(60),AMW(60),CE(20,60),CC(5,60)          CHEM
      DIMENSION R( 7, 7),B( 7,1),YINT(20),FY(20),PI(7),FSUM(20),YSUM(20)CHEM
     1 ,X(20),DELT(20),XLAM(20)                                             CHEM
      DIMENSION E(5),BB(5),Y(20)                                            CHEM
    5 CONTINUE                                                              CHEM
C                                                                           CHEM
```

```
      MA=1                                                              CHEM 370
C                                                                       CHEM 380
C-----INITIAL GUESS FOR EQUILIBRIUM CALCULATIONS....                    CHEM 390
C                                                                       CHEM 400
      DO10I=1,NS                                                        CHEM 410
 10   Y(I) = CWALL(I)*AMW(NI)/XMW(I)                                    CHEM 420
C                                                                       CHEM 430
C-----COMPUTE THE SIZE OF THE MATRIX                                    CHEM 440
C                                                                       CHEM 450
      NA=MM+1                                                           CHEM 460
C                                                                       CHEM 470
C     NS=NUMBER OF SPECIES....                                          CHEM 480
C                                                                       CHEM 490
C     CRIT=CRITERIA FOR CONVERGENCE.                                    CHEM 500
C                                                                       CHEM 510
      DT=25.                                                            CHEM 520
      DT=200.                                                           CHEM 530
      CRIT =TOL                                                         CHEM 540
      XBETA=CRIT                                                        CHEM 550
      BETA=0.                                                           CHEM 560
      LL=NS+1                                                           CHEM 570
      TOLD=0.0                                                          CHEM 580
C                                                                       CHEM 590
C     THE REMAINDER OF THE PROGRAM COMPUTES EQUILIBRIUM COMPOSITIONS    CHEM 600
C     CORRESPONDING TO THE ELEMENTAL MASS FRACTIONS IN THE CC-ARRAY     CHEM 610
C     FROM POINT N = NI TO POINT N = NF.                                CHEM 620
C                                                                       CHEM 630
      DO500N=NI,NF                                                      CHEM 640
      KT=1                                                              CHEM 650
      T = TT(N)*TD                                                      CHEM 660
      P=PP(N)                                                           CHEM 670
      BETOLD=0.0                                                        CHEM 680
      SUM=0.0                                                           CHEM 690
      DO15I=1,MM                                                        CHEM 700
 15   SUM=SUM + CC(I,N)                                                 CHEM 710
      DO20 I=1,MM                                                       CHEM 720
```

```
      IF(CC(I,N).LT.1.CE-10)CC(I,N)=1.CE-10
 20   E(I)=CC(I,N)/SUM
C
      CALL ALTERY(E,Y,TOLD)
C
      TINCR=ABS(T-TOLD)
      IF(TINCR.LE.50.)GOTO1750
 22   NT=1
      DO25 J=1,MM
      BB(J)=0.0
      DO 25  I=1,NS
 25   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
C-----SET-UP THE R-MATRIX AND THE B-VECTOR....
C
 40   YBAR=0.
      DO50I=1,NS
   50 YBAR=YBAR+Y(I)
C
C     YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES
C
C
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES
C
      DO60I=1,NS
      FAC=Y(I)/YBAR
      IF(FAC.LT.1.E-73)FAC=1.E-73
 60   FY(I)=Y(I)*(C(I)+ALOG(FAC))
C
C-----PROCEED TO CONSTRUCT THE R MATRIX
C
```

```
C-----INITIALIZE TO ZERO....
C
      DO75J=1,NA
      DO75K=1,NA
 75   R(J,K)=0.0
C
      DO90J=1,MM
      DO90K=J,MM
      SUM=0.
      DO80I=1,NS
 80   SUM=SUM+AA(I,J)*AA(I,K)*Y(I)
      R(J,K)=SUM
 90   R(K,J)=SUM
C
      DO 103 K=1,MM
      SUM=0.
      DO 101 I=1,NS
  101 SUM=SUM+AA(I,K)*Y(I)
      R(K,NA)=SUM
      R(NA,K)=SUM
  103 CONTINUE
C
C ----PROCEED TO CALCULATE THE VECTOR B.
C
      DO140J=1,MM
      SUM=0.
      DO130I=1,NS
 130  SUM=SUM+AA(I,J)*FY(I)
 140  B(J,1)=SUM+BB(J)
C
      SUM=0.
      DO150I=1,NS
 150  SUM=SUM+FY(I)
      B(NA,1)=SUM
C
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,MA,NMAX)
 155   CONTINUE
C
       DO160I=1,NA
C
C      PI(I)=LAGRANGINA MULTIPLIERS
C
  160  PI(I)=B(I,1)
       U=PI(NA)
       XBAR=U*YBAR
C
C-----COMPUTE THE MOLES OF EACH SPECIE....
C
       DO170I=1,NS
 170   FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR
       DO200I=1,NS
       PSUM=0.
       DO180J=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
       DO215I=1,NS
       DELT(I)=X(I)-Y(I)
 215   BETA=BETA+ABS(DELT(I))
       IF(BETA.GT.BETOLD)GOTO216
       IF(BETA.LT.XBETA)GOTO800
 216   CONTINUE
C
```

```
C-----COMPUTE THE CONVERGENCE PARAMENTER XLAMBD
C
      XLAMBD=1.
      DO210 I=1,NS
      IF(ABS(DELT(I)).LT.1.0E-20)DELT(I)=0.0
      IF(DELT(I).GE.0.)GOTO210
      IF(X(I).GT.0.)GOTO210
      XLAM(I)=-Y(I)/DELT(I)
      XLAMBD=AMIN1(XLAMBD,XLAM(I))
      XLAMBD=.99*XLAMBD
  210 CONTINUE
      XLAM1=XLAMBD
      IF(XLAM1.EQ.0.)XLAM1=1.0E-5
      DEBAR=0.
      DO220I=1,NS
  220 DEBAR=DEBAR+DELT(I)
C
C-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.
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
C-----DETERMINE THE FREE ENERGY GRADIENT.  IF POSITIVE REDUCE XLAMBDA
C     DFDL=FREE ENERGY GRADIENT
C
  230 DFDL=0.
      DO280I=1,NS
      FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)
      IF(FAC.LT.1.E-73)FAC=1.E-73
C260  DERP=(DELT(I)*YBAR-DEBAR*Y(I))/(YBAR+XLAMBD*DEBAR)
C280  DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC)) + DERP
  280 DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC))
      IF(DFDL.LT.0.000)GOTO300
      XLAMBD=.8*XLAMBD
```

```
      IF(XLAMBD.GT.1.0E-08)GOTO230                                      CHEM2170
C                                                                       CHEM2180
C-----THE VALUE OF XLAMBD THAT ASSURES CONVERGENCE HAS BEEN FOUND        CHEM2190
C                                                                       CHEM2200
 300  DO350I=1,NS                                                       CHEM2210
      IF(XLAMBD.GT.1.E-6)GOTO330                                        CHEM2220
      IF(DFDL.LT.0.)GOTO330                                             CHEM2230
      IF(XLAM1.LT.1.E-6)XLAM1=1.E-6                                     CHEM2240
C                                                                       CHEM2250
C-----CALCUALTE THE NEW COMPOSITION FOR THE NEXT ITERATION              CHEM2260
C                                                                       CHEM2270
      Y(I)=Y(I)+XLAM1*DELT(I)*.1                                        CHEM2280
      GOTO340                                                           CHEM2290
 330  Y(I)=Y(I)+XLAMBD*DELT(I)                                          CHEM2300
 340  IF(Y(I).LT.0.)Y(I)=1.E-73                                         CHEM2310
 350  CONTINUE                                                          CHEM2320
C                                                                       CHEM2330
 532  NT=NT+1                                                           CHEM2340
      BETOLD=BETA                                                       CHEM2350
      TOLD=T                                                            CHEM2360
C                                                                       CHEM2370
C-----IF THE NUMBER OF ITERATIONS EXCEED 900 STOP COMPUTATIONS          CHEM2380
C                                                                       CHEM2390
      IF(NT.GT.900)GOTO6000                                             CHEM2400
      GOTO40                                                            CHEM2410
 800  CONTINUE                                                          CHEM2420
C                                                                       CHEM2430
C-----CONVERT Y(I) TO MOLE FRACTIONS.....                               CHEM2440
C                                                                       CHEM2450
C     CONVERT EQUILIBRIUM MOLE FRACTIONS TO MASS FRACTIONS AND STORE    CHEM2460
C     THESE VALUES IN THE CE-MATRIX.  AMW(N) IS THE AVERAGE MOLECULAR   CHEM2470
C     WEIGHT AT THE POINT, N.                                           CHEM2480
C                                                                       CHEM2490
      SUMY=0.0                                                          CHEM2500
      DO900I=1,NS                                                       CHEM2510
 900  SUMY=SUMY+Y(I)                                                    CHEM2520
```

```
      IF(KT.GT.1)GOTO1500
      AMW(N) = 0.0
      DO1000I=1,NS
      Y(I)=Y(I)/SUMY
 1000 AMW(N) = AMW(N) + Y(I)*XMW(I)
      DO1005I=1,NS
 1005 CE(I,N) = Y(I)*XMW(I)/AMW(N)
      GOTO1800
C
C-----COMPUTE THE PARTIAL DERIVATIVE OF THE MOLE FRACTION, DYDT...
C
 1500 AMPLUS=0.0
      DO1525I=1,NS
      Y(I)=Y(I)/SUMY
 1525 AMPLUS=AMPLUS + Y(I)*XMW(I)
      DO1550I=1,NS
      DYDT(I,N)=0.0
      IF(Y(I).LT.1.0E-10)GOTO1550
      YY=Y(I)*AMW(N)/AMPLUS - CE(I,N)*AMW(N)/XMW(I)
      DYDT(I,N)=YY/DT
 1550 CONTINUE
      GOTO3300
C
C-----IF THE TEMPERATURE CHANGE IS LESS THAN 50 DEGREES FROM LAST
C     F. E. M.  CALCULATION ASSUME CURRENT VALUES AS EQUAL TO LAST
C     VALUES...
C
 1750 DO1760I=1,NS
      CE(I,N)=CE(I,N-1)
 1760 DYDT(I,N)=DYDT(I,N-1)
      AMW(N)=AMW(N-1)
 1800 CONTINUE
C
C     OPTIONAL OUTPUT OF POSITION , TEMPERATURE AND EQUILIBRIUM
C     COMPOSITIONS.
C
```

```
      IF(NDBUG.LT.2)GOTO3000                                              CHEM2890
      PRINT 2000,P,T     ,NT                                              CHEM2900
 2000 FORMAT(//,'  P = ',F5.3,' T(OK) = ',F6.0,5X,'NUMBER OF ITERATIONS CHEM2910
     X='I3,//,11X,'Y(I)',12X,'C(I,N)',/)                                  CHEM2920
      PRINT 2005,(SP(I),Y(I),CE(I,N),I=1,NS)                              CHEM2930
 2005 FORMAT(1X,A4,2E18.8)                                                CHEM2940
C                                                                         CHEM2950
 3000 CONTINUE                                                            CHEM2960
      KT=2                                                                CHEM2970
      T=T+DT                                                              CHEM2980
      IF(TINCR.GT.50.)GOTO22                                              CHEM2990
 3300 XBETA=CRIT                                                          CHEM3000
 5000 CONTINUE                                                            CHEM3010
 8000 CONTINUE                                                            CHEM3020
      RETURN                                                              CHEM3030
 6000 PRINT6001                                                           CHEM3040
 6001 FORMAT( ' NUMBER OF ITERATIONS EXCEEDED 900, PROGRAM TERMINATING')CHEM3050
      RETURN                                                              CHEM3060
      END                                                                 CHEM3070
```

```
      SUBROUTINE ALTERY(E,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 /SP1/SS,TOL,NDBUG
      DIMENSION E(5),Y(20),B(5),EOLD(5)
      DATA EOLD/5*0.0/
C
C-----CHECK TO SEE IF ELEMENTAL COMPOSITION HAS CHANGED SIGNIFICANTLY.
C     IF NOT, THEN RETURN....
C
      CHANGE=0.0
      DO5J=1,NE
      CHANGE=CHANGE+ABS(EOLD(J)-E(J))
  5   EOLD(J)=E(J)
      IF(CHANGE.LT.1.0E-3)RETURN
      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 CPMPOS
C     DISTRIBUTION AND THE MAXIMUM POSSIBLE MOLECULAR WEIGHT......
C
      DO20J=1,NE
      IF(E(J).GT.1.0E-8)GOTO20
      DO15I=1,NSP
      IF(AA(I,J).LE.0.0)GOTO15
      Y(I)=1.0E-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
C     FIRST GUESS.  ADJUST THE COMPOSITION OF EACH ELEMENT-SPECIE AS
```

```
C       REQUIRED......
C
        DO30J=1,NE
        B(J)=0.0
        DO30I=1,NSP
 30     B(J)=B(J)+AA(I,J)*Y(I)
        DO40J=1,NE
 40     Y(LSP(J))=Y(LSP(J)) + (E(J)-B(J))
        TOLD=0.0
        RETURN
        END
```

```
      SUBROUTINE THERMO(T,P)
C
C
C-----SUBROUTINE THERMO CALCULATES THE FREE ENERGY FUNCTION FOR EACH
C     CHEMICAL SPECIE.
C
C
      COMMON/NUMBER/NQ  ,NNS,NE,NC
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/EQ2/AA(20,5),ICODE(20)
      COMMON/THERM1/C(20),FORT(20)
C
C     T=TEMPERATURE IN OK
C
      T1=T
      T2=T1*T
      T3=T2*T
      T4=T3*T
      T5=T4*T
C
C
C-----CALCUALTE THE FREE ENERGY FUNCTION FORT(I)
C
C     FORT(I)=FREE ENERGY FUNCTION
C
      DO 41 I=1,NQ
      IF(T.GT.6000.   )GOTO6205
      FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.
     1        -EI(I)*T4/20.+FI(I)/T-GI(I)
      IF(ICODE(I).EQ.1)GOTO41
      C(I)=FORT(I)+ALOG(P)
      GOTO41
 6205 FORT(I)=AII(I)*(1.-ALOG(T))-BII(I)*T/2.-CII(I)*T2/6.-DII(I)*T3/12.
     1        -EII(I)*T4/20.+FII(I)/T-GII(I)
      IF(ICODE(I).EQ.1)GOTO41
```

```
      C(I)=FORT(I)+ALOG(P)                                    THER 370
   41 CONTINUE                                                THER 380
      RETURN                                                  THER 390
      END                                                     THER 400
```

```
      SUBROUTINE PROPRT(NSP,NI,NF)
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C     SUBROUTINE FOR THE CALCULATION OF TRANSPORT AND THERMO-
C     DYNAMIC 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           RO(N).....DENSITY AT POINT N,   LBM/ FT**3
C           TT(N).....TEMPERATURE AT POINT N, DEG. K
C           CP(I).....HEAT CAPACITY, CAL/GMOLE-K
C           CPM(N)....MIXTURE HEAT CAPACITY AT TEMPERATURE, TT(N)
C           H(I)......ENTHALPY OF COMPONENT I, CAL/GMOLE
C           HM(N).....MIXTURE ENTHALPY AT TEMPERATURE TT(N)
C           VIS(I)....VISCOSITY OF COMPONENT I, LB/FT-SEC
C           VISM(N)...MIXTURE VISCOSITY AT TEMPERATURE, TT(N)
C           TC(I).....THERMAL CONDUCTIVITY, CAL/CM-SEC-K
C           TCM(N)....THERMAL CONDUCTIVITY OF THE MIXTURE AT TT(N)
      COMMON /BLOCK1/V1(20),V2(20),V3(20)
      COMMON/BLOCK3/K1(20),K2(20)
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM, NT
      COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON/PROP1/PI(60),PO(60),TT(60),AMW(60),C (20,60),CC(5,60)
      COMMON/PROP2/VISM(60),RM(60),TCM(60)
      COMMON/PROP3/CP(20,60),H(20,60),CPM(60),HM(60)
      COMMON /PH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON/WT/SMW(20),AAT(5)
      COMMON /YL/ET (60),YOND(60)
      COMMON /DY/ DYDT(20,60)
      COMMON /DIF/D(5, 60)
      DIMENSION PHI(20,20),YPHI(20),Y(20),TC(20),VIS(20)
      DIMENSION SAMW(2)
      REAL  MU,MUDZ
```

```
      REAL K1,K2
      DATA R /1.98716/
C
      R7R = .7608
      TOLD=0.0
      DO200N=NI,NF
      T1=TT(N) *TD
      DO30J=1,5
 30   D(J,N)=0.8128E-07*(T1**1.659)/(PI(N)*RAD*UINF)
      PO(N) = R7R *PI(N)*AMW(N)/T1
      IF(ABS(T1-TOLD).LE.150.)GOTO150
      AA=.130E-7 + 3.35E-12*T1
      D12=AA*929.*(T1**1.659)/PI(N)
      T2=T1*T1
      T3=T2*T1
      T4=T3*T1
      T5=T4*T1
      DO90I=1,NSP
      IF(T1.GT.6000.)GOTO50
      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.
     X                  + EI(I)*T5/5.+ FI(I))*R
      GOTO60
 50   CP(I,N)=(AII(I)+BII(I)*T1+CII(I)*T2+DII(I)*T3+EII(I)*T4)*R
      H(I,N)=(AII(I)*T1+BII(I)*T2/2.+CII(I)*T3/3.+DII(I)*T4/4.
     X                  +EII(I)*T5/5.+FII(I))*R
 60   Y(I)=C(I,N)*AMW(N)/SMW(I)
      VIS(I)=(V1(I) + V2(I)*T1 + V3(I)*T2)*1.0E-05
      TC(I)=(K1(I)+K2(I)*T1)*1.0E-4/.662
 90   CONTINUE
C
C-----CALCULATE PHI(I,J) PARAMETERS FOR MIXTURE PROPERTIES....
C
      DO95I=1,NSP
      DO95J=1,NSP
      VIS12=SQRT(VIS(I)/VIS(J))
```

```
      SMW14=(SMW(J)/SMW(I))**.25
      PHI(I,J)=.354*((1.+VIS12*SMW14)**2)/SQRT(1.+SMW(I)/SMW(J))
   95 CONTINUE
C
C-----CALCULATION OF  MIXTURE  PROPERTIES...
C
      DO100I=1,NSP
      YPHI(I)=0.0
      DO100J=1,NSP
  100 YPHI(I)=YPHI(I)  +  Y(J)*PHI(I,J)
      VISM(N)=0.0
      HM(N)=0.0
      TCF=0.0
      CPF=0.0
      CPR=0.0
      SUMY=0.0
      DO120I=1,NSP
      IF(Y(I).LT.1.E-5)  GO  TO  120
      HM(N)=HM(N)+Y(I)*H(I,N)
      SUMY=SUMY+Y(I)
      CPF=CPF  +  Y(I)*CP(I,N)
      CPR=CPR  +          H(I,N)*DYDT(I,N)
      VISM(N)=VISM(N)+Y(I)*VIS(I)/YPHI(I)
      TCF=TCF  +  Y(I)*TC(I)/YPHI(I)
  120 CONTINUE
      CPM(N)=CPF  +  CPR
      TCR=RO(N)*D12*CPR/(AMW(N)*62.4)
      TCM(N)=TCF  +  TCR
C     PR=VISM(N)*CPM(N)*14.88/(TCM(N)*AMW(N))
      TOLD=T1
      GOTO200
  150 CONTINUE
      DO160I=1,NSP
      CP(I,N)=CP(I,N-1)
  160 H(I,N)=H(I,N-1)
      VISM(N)=VISM(N-1)
```

```
      TCM(N)=TCM(N-1)                                                   PROP1100
      CPM(N)=CPM(N-1)                                                   PROP1110
  200 CONTINUE                                                          PROP1120
C                                                                       PROP1130
C----- NONDIMENSIONALIZE QUANTITIES -----                               PROP1140
C                                                                       PROP1150
      MUDZ=VISM(NF)                                                     PROP1160
      DO 250 I=NI,NF                                                    PROP1190
      T1=TT(I)*TD                                                       PROP1200
      VISM(I) = VISM(I)/MUDZ                                            PROP1210
      TCM(I) = TCM(I)*AKNF*6.715E-2                                     PROP1220
      RO(I) = RO(I)/(RDZ*32.174)                                        PROP1230
      RM(I)=RO(I)*VISM(I)                                               PROP1240
      CPM(I)=CPM(I)*CPNF/AMW(I)                                         PROP1250
      DO 250 K=1,NSP                                                    PROP1280
      CP(K,I) = CP(K,I)*CPNF/SMW(K)                                     PROP1290
      H(K,I) = H(K,I)*HNF*1.89/SMW(K)                                   PROP1300
  250 CONTINUE                                                          PROP1310
      RETURN                                                            PROP1320
      END                                                               PROP1330
```

```
      SUBROUTINE GAS (KODE )
C
C     **   THERMODYNAMIC AND TRANSPORT PROPERTIES OF AIR **
C     **  REFERENCE NASA TR R-50 **
C
C THE FOLLOWING PROPERTIES ARE CALCULATED
C                   TEMPERATURE AT WHICH PROPERTIES ARE WANTED (T) IN DEG R
C                   PRESSURE AT WHICH PROPERTIES ARE WANTED (P) IN LB/IN**2
C                   RATIO OF SPECIFIC HEATS (GAMMA) IN DIMENSIONLESS
C                   SPECIFIC HEAT AT CONSTANT PRESSURE (CP) IN BTU/LB-DEG R
C                   ABSOLUTE VISCOSITY (V) IN LB/FT-SEC
C                   PRANDTL NUMBER (PR) IN DIMENSIONLESS
C                   THERMAL CONDUCTIVITY (XK) IN BTU/FT-SEC-DEG R
C                   PRESSURE (P) IN ATMOSPHERES
C                   DENSITY (DEN) IN LB/FT**3
C                    ENTHALPY (H) IN BTU/LB
C                    ENTROPY (S) IN BTU/LB-DEG R
C                    COMPRESSIBILITY (Z) IN DIMENSIONLESS
C                    SPEED OF SOUND (SOS) IN FT/SEC
C                    SPECIFIC HEAT AT CONSTANT VOLUMN (CV) IN BTU/LB-DEG R
C                    ENTROPY (S) IN FT**2/SEC**2
C                    VELOCITY (VEL) IN FT/SEC
C                    PRESSURE (P) IN LBS/FT**2
C                    MACH NUMBER (M) IN DIMENSIONLESS
C
C
C NOMENCLATURE    1=OXYGEN MOLECULES, 2=NITROGEN MOLECULES, 3=OXYGEN ATMOS
C                 4=NITROGEN ATMOS, 5=OXYGEN IONS, 6=NITROGEN IONS
C                 7=ELECTRONS
C
C
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON/PROP1/FI(60),RHO(60),TI(60),AMW(50),C (20,60),CC(5,60)
      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/RVW,PRW,TWOLD,FLUX(20),CWALL(20),ECWALL(5)
      REAL  MU,MUDZ
      LOGICAL MCONV,GCONV,SCONV
      DATA GASC /49721.7/
C
C
      DO 2000 I=KODE,NETA
      T = TI(I) * TD
      P = PI(I)
C
C THE FOLLOWING PART OF PROGRAM USES PRESSURE IN ATMOSPHERES
C AND TEMPERATURE IN DEG K
C
      ITER=0
C
C     **  TEMPERATURE - ENTHALPY ITERATION   **
C
  900 CONTINUE
      ITER=ITER+1
      IF(T.LT.100.) T=100.
      A1=11390./T
      A2=18990./T
      A3=2270./T
      A4=3390./T
      A5=228./T
      A6=326./T
      A7=22800./T
      A8=48600./T
      A9=27700./T
      A10=41500./T
      A11=38600./T
      A12=58200./T
      A13=70.6/T
      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
      TSQRT=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.*AA1*A1+AA2*A2)/(3.+2.*AA1+AA2))+(A3/(AA3-1.))
      E2=2.5+ (A4/(AA4-1.))
      E3=1.5+((3.*AA5*A5+AA6*A6+5.*AA7*A7+AA8*A8)/(5.+3.*AA5+AA6+5.*AA7+
     1AA9))
```

```
      E4=1.5+((10.* AA9*A9+6.*AA10*A10)/(4.+10.*AA9+6.*AA10))
      E5=1.5+((10.*AA11*A11+6.*AA12*A12)/(4.+10.*AA11+6.*AA12))
      E6=1.5+((3.*AA13*A13+5.*AA14*A14+5.*AA15*A15+AA16*A16+5.*AA17*A17)
     1/(1.+3.*AA13+5.*AA14+5.*AA15+AA16+5.*AA17))
      E7=1.5
C TOTAL ENERGY PER COMPONENT OF GAS MIXTURE
      EN1=E1
      EN2=ET
      EN3=E3+29500./T
      EN4=E4+56600./T
      EN5=E5+187500./T
      EN6=E6+225400./T
      EN7=E7
C LOGS OF PARTITION FUNCTIONS
      TL1=ALOG(T)*3.5
      TL2=ALOG(T)*2.5
      EQ1=TL1+.11+ALOG((3.+2.*AA1+AA2)/(1.-(1.0/AA3)))
      EQ2=TL1-.42-ALOG((1.-(1.0/AA4)))
      EQ3=TL2+.5+ALOG((5.+3.*AA5+AA6+5.*AA7+AA8))
       EQ4=TL2+.3+ALOG((4.+10.*AA9+6.*AA10))
      EQ5=TL2+.5+ALOG((4.+10.*AA11+6.*AA12))
       EQ6=TL2+.3+ALOG((1.+3.*AA13+5.*AA14+5.*AA15+AA16+5.*AA17))
      EQ7=TL2-14.24
C EQUILIBRIUM CONSTANS FOR CHEMICAL REACTIONS
      EK1=-59000./T+2.*EQ3-EQ1
      EK2=-113200./T+2.*EQ4-EQ2
      EK3=-158000./T+EQ5+EQ7-EQ3
      EK4=-168800./T+EQ6+EQ7-EQ4
      CCC=-79.9
      IF(EK1.LE.CCC) EK1=-79.9
      IF(EK2.LE.CCC) EK2=-79.9
      IF(EK3.LE.CCC) EK3=-79.9
      IF(EK4.LE.CCC) EK4=-79.9
      XK1=EXP(EK1)
      XK2=EXP(EK2)
      XK3=EXP(EK3)
```

```
      XK4=EXP(EK4)                                                      GAS 1450
      XK34=.2*XK3+.8*XK4                                                GAS 1460
      EE1=(-0.8+(.64+.6*(1.+((4.*P)/XK1)))**0.5)/(2.*(1.+4.*P/XK1))     GAS 1470
      EE2=(-0.4+(.16+3.84*(1.+(4.*P)/(XK2)))**0.5)/(2.*(1.+4.*P/XK2))   GAS 1480
      EE3= 1./(( 1.+P/XK34)**.5)                                        GAS 1490
C COMPRESSIBILITY (Z) DIMENSIONLESS                                     GAS 1500
      Z=1.+EE1+EE2+2.*EE3                                               GAS 1510
C COMPONENT MOL FRACTIONS IN AIR                                        GAS 1520
      X1=(.2-EE1)/Z                                                     GAS 1530
      X2=(.8-EE2)/Z                                                     GAS 1540
      X3=(2.*EE1-.4*EE3)/Z                                              GAS 1550
      X4=(2.*EE2-1.6*EE3)/Z                                             GAS 1560
      X5= .4*EE3/Z                                                      GAS 1570
      X6= 1.6*EE3/Z                                                     GAS 1580
      X7= 2.*EE3/Z                                                      GAS 1590
      IF(X1.LE.0.)  X1=1.E-20                                           GAS 1600
      IF(X2.LE.0.)  X2=1.E-20                                           GAS 1610
      IF(X3.LE.0.)  X3=1.E-20                                           GAS 1620
      IF(X4.LE.0.)  X4=1.E-20                                           GAS 1630
      IF(X5.LE.0.)  X5=1.E-20                                           GAS 1640
      IF(X6.LE.0.)  X6=1.E-20                                           GAS 1650
      IF(X7.LE.0.)  X7=1.E-20                                           GAS 1660
C ENERGY PER MOL OF INITIALLY UNDISSOCIATED AIR-DIMENSIONLESS           GAS 1670
      ER= Z*(X1*EN1+X2*EN2+X3*EN3+X4*EN4+X5*EN5+X6*EN6+X7*EN7)          GAS 1680
C ENTHALPY PER INITIAL MOL OF AIR-DIMENSIONLESS                         GAS 1690
      HR=ER+Z                                                           GAS 1700
C ENTHALPY PER INITIAL MOL OF AIR (H) IN BTU/LB                         GAS 1710
      H=HR*T*.12348                                                     GAS 1720
      IF(KODE.LT.NETA) GO TO 1060                                       GAS 1730
      HRATO=.5*(H-HD)/H                                                 GAS 1740
      AHR   = ABS( HRATO )                                              GAS 1750
      IF(AHR .LE. 0.0010) GO TO 999                                     GAS 1760
      IF(ITER .GT.1) GO TO 203                                          GAS 1770
      TP=T                                                              GAS 1780
      HP=HRATO                                                          GAS 1790
      T = T *(1. - HRATO )                                              GAS 1800
```

```
      IF(ITER .LT. 15) GO TO 900
 203  CONTINUE
      TS=T*(1.0-HRATO)
      IF(HRATO*HP .LT.0.0) TS=.5*(T+TP)
      TP=T
      T=TS
      HP=HRATO
      IF(ITER .LT. 15) GO TO 900
      WRITE(6,200) T,H,HT
 200  FORMAT(39H1TEMPERATURE-ENTHALPY DID NOT CONVERGE /3E15.6)
C     CALL OUTPUT(4)
      STOP
 999  CONTINUE
      TD = T
C
 1000 CONTINUE
C ENTROPY PER INITIAL MOL OF AIR-DIMENSIONLESS
      D1=EQ1+E1+1.
      D2=EQ2+ET+1.
      D3=EQ3+E3+1.
      D4=EQ4+E4+1.
      D5=EQ5+E5+1.
      D6=EQ6+E6+1.
      D7=EQ7+E7+1.
C TOTAL ENTROPY
      SR=Z*(X1*D1+X2*D2+X3*D3+X4*D4+X5*D5+X6*D6+X7*D7)-Z*(X1*ALOG(X1) +
     1X2*ALOG(X2)+X3*ALOG(X3)+X4*ALOG(X4)+X5*ALOG(X5)+X6*ALOG(X6)+X7*
     2ALOG(X7))-Z*ALOG(P)
C ENTROPY PER INITIAL MOL OF AIR (S) IN BTU/LB-DEG R
      S    =SR*0.0686
C SPECIFIC HEAT AT CONSTANT VOLUME-CV
      FF1=3.+2.*AA1+AA2
      CV1=2.5+((2.*AA1*A1*A1+AA2*A2*A2)/FF1)-(((2.*AA1*A1+AA2*A2)/FF1)**
     12.)+((.25*A3*A3)/(((2.*A19)/(1.-A19*A19))**2))
      CV2=2.5+((.25*A4*A4)/(((2.*A21)/(1.-A21*A21))**2))
      CV3=1.5+((3.*AA5*A5*A5+AA6*A6*A6+5.*AA7*A7*A7+AA8*A8*A8)/(5.+3.*AA
```

```
     15+AA6+5.*AA7+AA8))-((E3-1.5)**2.)                                 GAS 2170
      CV4=1.5+((10.*AA9*A9*A9+6.*AA10*A10*A10)/(4.+10.*AA9+6.*AA10))    GAS 2180
     1-((E4-1.5)**2.)                                                   GAS 2190
      CV5=1.5+((10.*AA11*A11*A11+6.*AA12*A12*A12)/(4.+10.*AA11+6.*AA12))GAS 2200
     1-((E5-1.5)**2.)                                                   GAS 2210
      CV6=1.5+((3.*AA13*A13*A13+5.*AA14*A14*A14+5.*AA15*A15*A15+AA16*A16GAS 2220
     1*A16+5.*AA17*A17**2)/(1.+3.*AA13+5.*AA14+5.*AA15+AA16+5.*AA17))-((GAS 2230
     2E6-1.5)**2.)                                                      GAS 2240
      CV7=1.5                                                           GAS 2250
C LOGARITHMIC DERIVATIVES                                               GAS 2260
      CK1=TT*(59000./T+2.*E3-E1)                                        GAS 2270
      CK2=TT*(113200./T+2.*E4-ET)                                       GAS 2280
      CK3=TT*(158000./T+E5+E7-E3)                                       GAS 2290
      CK4=TT*(168800./T+E6+E7-E4)                                       GAS 2300
      CK34=.2*CK3+.8*CK4                                                GAS 2310
      PK1= CK1+TT                                                       GAS 2320
      PK2= CK2+TT                                                       GAS 2330
      PK3= CK3+TT                                                       GAS 2340
      PK4= CK4+TT                                                       GAS 2350
      PK34=0.2*PK3+0.8*PK4                                              GAS 2360
C PARTIAL DERIVATIVES REQUIRED FOR CP                                   GAS 2370
      DE1P=(PK1*EE1*(1.+EE1)*(.2-EE1))/(.8*(.5-EE1))                    GAS 2380
      DE2P=(PK2*EE2*(1.2+EE2)*(.8-EE2))/(.4*(4.8-EE2))                  GAS 2390
      DE3P=.5*PK34*EE3*(1.-EE3**2)                                      GAS 2400
      DZX1P=-DE1P                                                       GAS 2410
      DZX2P=-DE2P                                                       GAS 2420
      DZX3P=2.*DE1P - .4*DE3P                                           GAS 2430
      DZX4P=2.*DE2P-1.6*DE3P                                            GAS 2440
      DZX5P=.4*DE3P                                                     GAS 2450
      DZX6P=1.6*DE3P                                                    GAS 2460
      DZX7P=2.* DE3P                                                    GAS 2470
C EQUATION FOR SPECIFIC HEAT AT CONSTANT PRESSURE                       GAS 2480
      CPF=Z*(X1*(CV1+1.)+X2*(CV2+1.)+X3*(CV3+1.)+X4*(CV4+1.)+X5*(CV5+1. GAS 2490
     1)+X6*(CV6+1.)+X7*(CV7+1.))                                        GAS 2500
      CPR = CPF +            T*(DZX1P*(EN1+1.)+DZX2P*(EN2+1.)+DZX3P*(EGAS 2510
     2N3+1.)+DZX4P*(EN4+1.)+DZX5P*(EN5+1.)+DZX6P*(EN6+1.)+DZX7P*(EN7+1.)GAS 2520
```

```
    4)
      CPF = CPP
C SPECIFIC HEAT AT CONSTANT  PRESSURE (CP) IN BTU/LB-DEG R
      CP=CPR*.0686
      CPF = CPF*.0686
C DENSITY (DEN) IN LB/FT**3
      DEN=22.03703*P/(Z*T)
C **TRANSPORT PROPERTIES**
C COLLISION CROSS SECTIONS
      S2=31.4*1.E-16*(1.+(112./T))
      SI2=(S2/3.1415927)**.5
      SI4=(1.11676-(.01490* ALOG(1.-(1.-A23) **.5))-(.23654* ALOG
     1(1.-(1.-A24)**.5))-(.11582* ALOG(1.-(1.-A25)**.5)))*1.0E-8
      S4=3.1415927*(SI4)**2
      SI24=(SI2+SI4)/2.
      S24=3.1415927*(SI24)**2
      S47=9.40*1.0E-14/TSQRT
      FI=ALOG(1.042*1.0E-7*TSQ*(P*X7 )**(-.5))
      S7=8.55644*1.CE-6*(1./TSQ)*FI
      SIP4=(1.11676-(.0149*ALOG(1.-(1.-2.*A23)**.5))-(.23654*ALOG(1.-(1.
     1-2.*A24)**.5))-(.11582* ALOG(1.-(1.-2.*A25)**.5)))*1.0E-8
      SP4=3.145927*(SIP4)**2
      SIP24=(SI2+SIP4)/2.
      SP24=3.145927*SIP24**2
C COMPONENT MOL FRACTIONS FOR INDEPENDENT REACTIONS
      F1=1.+EE1
      F2=1.2+EE2
      F3=1.+EE3
      X1OD=(.2-EE1)/F1
      X2OD=.3/F1
      X3OD=2.*EE1/F1
      X2ND=(.8-EE2)/F2
      X3ND=.4/F2
      X4ND=2.*EE2/F2
      X4I=(1.-EE3)/F3
      X6I=EE3/F3
```

```
C MEAN FREE PATH RATIOS
      SS1=S24/S2
      SS2=S4/S2
      SS3=S7/S2
      SS4=S47/S2
      FP1OD=X1OD+X2OD*.9660918 +X3OD*SS1*.8164966
      FP2OD=X1OD*1.032796+X2OD+X3OD*SS1*.8528029
      FP3OD=X1OD*1.154701*SS1+X2ND*SS1*1.128152+X3OD*SS2
      FP2ND=X2ND+X4ND*SS1*.8164966+X3ND*SS1*.8528029
      FP3ND=X2ND*SS1*1.128152+X4ND*SS2*.9660918+X3ND*SS2
      FP4ND=X2ND*SS1*1.154701+X4ND*SS2+X3ND*SS2*1.032796
      FP4I=X4I*SS2+X6I*SS2
      FP6I=X4I*SS2+X6I*SS3
      FP7I=X4I*SS4*1.414186+X6I*SS3*1.414186+X6I*SS3
C VISCOSTITES OF THE COMPONENTS FOR THE DIFFERENT REACTIONS
      V1OD=1.054093*X1OD*1./FP1OD
      V2OD=.9860133*X2OD*1./FP2OD
      V3OD=.745356*X3OD*1./FP3OD
      V2ND=.9860133*X2ND*1./FP2ND
      V3ND=.745356*X3ND*1./FP3ND
      V4ND=.6972167*X4ND*1./FP4ND
      V4I=.6972167*X4I*1./FP4I
      V6I=.6972167*X6I*1./FP6I
      V7I=.4367848*1.0E-2*X6I*1./FP7I
      VROD=V1OD+V2OD+V3OD
      VRND=V2ND+V3ND+V4ND
      VRI=V4I+V6I+V7I
      F4=EE2/(.2-EE1+EE2)
      F5=2.*EE3/(.8-EE2+2.*EE3)
      VR=VROD+(F4*(VRND-VROD))+(F5*(VRI-VRND))
C TOTAL VISCOSITY (V) IN LB/FT-SEC
      V=VR*.9841838*1.0E-6*TSQRT/(1.+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*CV6+.4736842
      G6=.2105363*CV7+.4736842
      XKNOD=(V1OD*.9*G1)+(V2OD*1.028571*G2)+(V3OD*1.8*G3)
      XKNND=(V2ND*1.028571*G2)+(V3ND*1.8*G3)+(V4ND*2.057143*G4)
      XKNI=(V4I*2.057143*G4)+(V6I*2.057143*G5)+(V7I*52416.0*G6)
      XKN=XKNOD+(F4*(XKNND-XKNOD))+(F5*(XKNI-XKNND))
C CONDUCTIVITY DUE TO CHECMICAL REACTIONS FOR THE DIFFERENT REACTIONS
      XKROD=(.178637*(T*PK1)**2)/((SP24/(1.732051*S2))*(((X3OD+2.*X1OD)
     1**2)/(X3OD*X1OD)+(4.*X2OD/X3OD))+(X2OD/(1.414214*X1OD)))
      XKRND=(.178637*(T*PK2)**2)/((SP24/(1.732051*S2))*((((X4ND+2.*X2ND)
     1**2)/(X4ND*X2ND))+(X3ND/X2ND)) +(SP4*2.*X3ND/(S2*X4ND)))
      XKR1=(.178637*(T*PK34)**2)/(((.5*SP4/S2)+(.4347826*1.0E-2*S47/S2))
     1*((X4I+X6I)**2)/(X4I*X6I))
      XKOD=XKNOD+XKROD
      XKND=XKNND+XKRND
      XKI=XKNI+XKR1
      XKR=XKOD+(F4*(XKND-XKOD))+(F5*(XKI-XKND))
C TOTAL THERMAL CONDUCTIVITY (XK) IN BTU/FT-SEC-DEG R
      XK=XKR*((.3206522*1.0E-6*TSQRT)/(1.+A22))
C PRANDTL NUMBER (PR) DIMENSIONLESS
      PRN = .2105263 * CPR * VR / XKR
      IF(I.EQ. 1) PRW = PRN
C FORM REQUIRED BY CALL STATEMENT
C
C     **  RHO UNITS SLUGS/FT**3
C     **  MU UNITS LBM/FT-SEC
C     **  RM UNITS LBF**2 SEC**3/FT**6
C
      MU (I) = V
      RHO(I)=DEN/32.174
      RM(I)=RHO(I)*MU(I  )/32.174
      AK(I) = XK
      CPT(I) = CPF
C *** CALCULATE  THE MEAN MOLECULAR WT. ***
      REAL = 25050.*S    *Z / SR
```

```
      AMW(I)= GASC / REAL
C 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(6,I) = X6     *14.00/AMW(I)
      C(5,I) = X5     *16.00/AMW(I)
      C(7,I) = X7     /(1820.*AMW(I))
C 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
C
      DO 40 I=KODE,NETA
C
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
C
 40   CONTINUE
 100  FORMAT(1X,9E14.6)
      RETURN
      END
```

```
      SUBROUTINE EFLUX
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON /R4/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON /RFLUX/ F(60),IRAD,ITYPE
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(50),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. * PL +13800.
      IF (TS -TSI ) 300,200,200
 200  EP = 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
 400  E(I) =E(I) *RZB
C     IF(IEM.GT.1) E(I) = .6 *E(I) +.4 *EOLD(I)
C
C  **** E IS NONDIMENSIONAL  ***
C
 100  CONTINUE
      RETURN
      END
```

```
      SUBROUTINE TRANS (ISW)
C
C-----THIS IS A MODIFIED VERSION OF SUBROUTINE TRANS FROM K WILSON
C     TRANS IS DOCUMMENTED IN  LMSC-687209 APRIL 69  ----------------
C
      COMMON /ZPI/ ZPO(6), ZPN(6),ZPH(2),  ZPC(7)
      COMMON /FINV/ NHVL,NIHVC,FHVC(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/PROP1/P (60),  R(60), T(60),AMW(50),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,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,   IDG,MCONV,ECONV,DCONV,LT,IAB
      COMMON /RFLUX/ E(60),IRAD,ITYPE
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON/WT/SMW(20),AWT(5)
      COMMON /TEST/ETZ(60),IEZ
      COMMON /NUMDEN/ SNDO2(60), SNDN2(60), SNDO(60), SNDN(60),
     1                                     SNDE(60), SNDC(60),
     2              SNDH(60), SNDC2(60), SNDH2(60), SNDCO(60),
     3              SNDC3(60),SNDC2H(60)
      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)
      COMMON /SPEC/ MF, XMOL
```

```
      DIMENSION  XKT(60),          DQ(60)
C
C **   BAND AVERAGE ABSORPTION CROSS SECTION (EQ.A2)   **
C
      SIGMA(ZH,ZA,ZB,ZG)=  ((5.0E+03*T1*ZG*ZKZ)/BE) * (EXP(ZDL/T1)
     1                      *ZH*(ZA+ZB* (ZH**2)/3.0) +
     2                      T1 * (ZA+2.0*ZB*T12) -T1*EXP((ZH-ZHVP)/T1)
     3                      *(ZA+ZB*(ZHVP-ZH)**2) -T1*EXP((ZH-ZHVP)/T1)
     4                      *2.0*ZB*T1*(ZHVP-ZH+T1))
      SIGMA2(ZH,ZG,ZE,ZY)=7.26E-16*T1*ZG*EXP((-ZE+ZY+ZDL)/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)
C
C **   W(GROUP)/D CORRELATION (EQ.88)   **
C
      PHI1(ZX)=(ATAN(1.570796 *ZX)/1.570796 )
C
C **   FLUX DIVERGENCE OVERLAPPING FUNCTION (EQ.92)   **
C
      PHI2(ZX)=EXP(-ZX)
C
      DO 400 I=1,NES
  400 T(I)= T(I)*TD
      ZHVP=5.0
      YI=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**(2.0/7.0))/((T(NES)/11606.)**(1.0/7.0))
      ZDL=AMIN1(0.20,FNE)
C
C **   DEBUG PRINT   **
C
      IF (IDG.NE.0) CALL BUGPR (1)
      DELTA=W(1) * XL * 30.4806
      CALL BUGPR (2)
```

```
 6001 CONTINUE
      DO 91 L=1,NES
      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).GT.15000.) GO TO 6
C
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=11.79563 -0.317964 * T(L)/1.0E3 + 0.013765 * (T(L)/1.0E3)**2
    7 CONTINUE
      T12=T1**2
      GH = 6.4994
      DO 5 K=1,12
      GF=FHVC(K)/T1
      GHM=GH
      GH=EXP(-GF)  *GF  *  (GF**2 + 3.0 *GF  +6.0  + 6.0/GF)
C
C **   PLANK MEAN ABSORPTION COEFFICIENT FOR BAND INTERVALS (EQ.A3)  **
C
      DEEC(K,L)=5.04E3  *  (T12**2)  *  (GHM-GH)
```

```
      BE=BEFC(K,L)
C
C **    ABSORPTION CROSS SECTIONS   **
C       SPECIES --
C                    N        N2       CO
C                    O        O2
C                    C        C2       C2H
C                    H        H2       C3
C
      SGH=0.
      SGN=0.
      SGC=0.
      SGO=0.
      SGCO=0.
      SGC2=0.
      SGO2=0.
      SGN2=0.
      SGH2=0.
      SGC3=0.
      SGC2H = 0.0
      GO TO (581,582,583,584,585,586,587,588,589,590,591,592),K
  581 SGH=SIGMA(2.4,1.0,0.0,1.0)  *  EXP(-13.56/T1)
      SGC=SIGMA(3.78,  0.3,   0.0488,  1.33)  * EXP(-11.26/T1)
      SGN=SIGMA(4.22,  0.24,  0.0426,  4.5) * EXP(-14.54/T1)
      SGO=SIGMA(4.22,  0.24,  0.0426,   .8888889)  * EXP(-13.61/T1)
      GO TO 38
  582 ZZHV=5.5
      SGC2=8.0E-18 * EXP(-0.5/T1)  +  3.0E-18
      SGC3=4.0E-18
  593 CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)
      SGC=SIGMA2(ZZHV, 1.33,  11.26,  3.78) * ZZC + SGC
      SGN=SIGMA2 (ZZHV,4.50,  14.54,  4.22) * ZZN
  594 SGO=SIGMA2 (ZZHV, .889,  13.61,  4.22) * ZZO
  595 SGH=SIGMA2 (ZZHV, 1.00,  13.56,  2.40)
      GO TO 38
  583 ZZHV=6.5
```

```
      SGC2=1.0E-18                                          TRAN1450
      SGCO=3.0E-18 * EXP(-0.7/T1)                           TRAN1460
      GO TO 593                                             TRAN1470
  584 ZZHV=7.5                                              TRAN1480
      SGC=5.0E-17  * EXP(-4.18/T1)/SUMC                     TRAN1490
      SGCO=1.9E-17  * EXP(-0.5/T1)                          TRAN1500
      SGO2=6.0E-19                                          TRAN1510
      SGC2H = 1.3E-18                                       TRAN1520
      GO TO 593                                             TRAN1530
  585 ZZHV=8.5                                              TRAN1540
      SGC=5.0E-17 *EXP(-4.18/T1)/SUMC  +                    TRAN1550
     1     2.2E-17* EXP(-2.68/T1)/SUMC                      TRAN1560
      SGCO=2.5E-17                                          TRAN1570
      SGO2=2.0E-19                                          TRAN1580
      SGC2H = 8.5E-19                                       TRAN1590
      GO TO 593                                             TRAN1600
  586 ZZHV=9.5                                              TRAN1610
      SGC=5.0E-17 * EXP(-4.18/T1)/SUMC  +                   TRAN1620
     1     2.2E-17 * EXP(-2.68/T1)/SUMC                     TRAN1630
      SGCO=5.0E-18                                          TRAN1640
      SGO2=1.0E-18                                          TRAN1650
      GO TO 593                                             TRAN1660
  587 SGN=3.2E-18 *T1  *EXP(-10.2/T1)/SUMN                  TRAN1670
      SGO2=6.0E-19                                          TRAN1680
      ZZHV=10.4                                             TRAN1690
      CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)                        TRAN1700
  596 SGC=(8.5E-17 *EXP(-1.26/T1)  +  2.2E-17 * EXP(-2.75/T1)   TRAN1710
     1     +  5.0E-17 * EXP(-4.18/T1))/SUMC                 TRAN1720
      GO TO 594                                             TRAN1730
  588 ZZHV=10.9                                             TRAN1740
      CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)                        TRAN1750
      SGN=(5.16E-17  *EXP(-3.56/T1))/SUMN                   TRAN1760
      GO TO 596                                             TRAN1770
  589 ZZHV=11.6                                             TRAN1780
      CALL ZHV(ZZHV,ZZO,ZZN,ZZI,ZZC)                        TRAN1790
      SGN2=1.0E-18                                          TRAN1800
```

```
      SGN=(5.16E-17 *  EXP(-3.50))/SUMN                                   TRAN1810
  598 SGC=(9.9E-17  +  8.5E-17 * EXP(-1.26/T1)  +2.2E-17 * EXP(-2.75/T1)TRAN1820
     1      +  5.0E-17 * EXP(-4.18/T1))/SUMC                               TRAN1830
      IF (K.LT.11) GO TO 594                                               TRAN1840
      GO TO 38                                                             TRAN1850
  590 ZZHV=12.7                                                            TRAN1860
      CALL ZHV  (ZZHV,ZZO,ZZN,ZZI,ZZC)                                     TRAN1870
      SGN2=2.0E-18                                                         TRAN1880
      SGH2 = 2.7E-17                                                       TRAN1890
  599 SGN=(6.4E-17 * EXP(-2.30/T1)  +  5.16E-17 * EXP(-3.50/T1))/SUMN     TRAN1900
     1      +  SGN                                                         TRAN1910
      GO TO 598                                                            TRAN1920
  591 SGH=1.18E-17/SUMH                                                    TRAN1930
      SGO=3.6E-17/SUMO                                                     TRAN1940
      SGN2=1.0E-17                                                         TRAN1950
      SGH2 = 2.7E-17                                                       TRAN1960
      GO TO 599                                                            TRAN1970
  592 SGN=3.6E-17/SUMN                                                     TRAN1980
      SGN2=1.0E-18                                                         TRAN1990
      GO TO 599                                                            TRAN2000
 '38  CONTINUE                                                             TRAN2010
      FMUC(K,L)= SNDH(L)*SGH + SNDC(L)*SGC + SNDN(L)*SGN + SNDO(L)*SGO     TRAN2020
     1           + XMOL *    (SNDN2(L)*SGN2 + SNDO2(L)*SGO2 +              TRAN2030
     2           SNDC2(L)*SGC2 + SNDH2(L)*SGH2 + SNDCO(L)*SGCO +           TRAN2040
     3           SNDC3(L)*SGC3 +SNDC2H(L)*SGC2H )                          TRAN2050
      IF (L.GT.1) GO TO 8                                                  TRAN2060
      TAUC(K,L)=0.                                                         TRAN2070
      GO TO 5                                                              TRAN2080
    8 TAUC(K,L)=TAUC(K,L-1)+(YD(L)-YD(L-1))*                               TRAN2090
     1      (FMUC(K,L-1)+FMUC(K,L)) * DELTA                                TRAN2100
    5 CONTINUE                                                             TRAN2110
      IF (LINES.EQ.0) GO TO 91                                             TRAN2120
C                                                                          TRAN2130
C **   FRACTIONAL POPULATION STATES FOR H, N, O, C  **                     TRAN2140
C                                                                          TRAN2150
      CALL ZP (T1,SUMN,SUMO,SUMH,SUMC)                                     TRAN2160
```

```
C **    CALCULATION OF PARAMETERS FOR 9 LINE GROUPES   **
C       WN -- NUMBER OF LINES
C       FG -- EFFECTIVE F-NUMBER
C       GP -- EFFECTIVE HALF-WIDTH
C
C GROUP 1
      FG(1,2)=(1.02 * ZPC(5)  +  .795 * ZPC(6)  +  0.114 * ZPC(7))
     1   /WN(1,2)
      GP(1,2)=(8.16E-11  * SQRT(ZPC(5))  +  1.25E-10 * SQRT(ZPC(6))
     1     +2.55E-10 * SQRT(ZPC(7)))**2 /(FG(1,2)* WN(1,2)**2)
      FG(1,3)=(1.040 * ZPN(4)  +  1.29 * ZPN(5)  +  0.00 *ZPN(6))
     1        /WN(1,3)
      GP(1,3)=(6.65E-11 * SQRT(ZPN(4))  +  1.71E-10 * SQRT(ZPN(5))
     1       +  0.00E-10 * SQRT(ZPN(6)))**2/(FG(1,3) * WN(1,3)**2)
      FG(1,4)=(1.00 * ZPO(5)  +  .978 * ZPO(6))/WN(1,4)
      GP(1,4)=(3.90E-11 * SQRT(ZPO(5))  +  9.58E-11 * SQRT(ZPO(6)))**2
     1        /(FG(1,4) * WN(1,4)**2)
      FMUL(1,L)=FMUC(1,L)
C GROUP 2
      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
     1        /(FG(2,2) * WN(2,2)**2)
      FG(2,3)=(0.047* ZPN(4)  +  2.85E-2 * ZPN(5))/WN(2,3)
      GP(2,3)=(1.11E-10 * SQRT(ZPN(4))  +  6.07E-11 * SQRT(ZPN(5)))**2
     1        /(FG(2,3) * WN(2,3)**2)
      FG(2,4)=(.0217 * ZPO(4)  +  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)   +  6.150 * ZPC(3))
     1         /WN(4,2)
      GP(4,2)=(9.57E-12 * SQRT(ZPC(1))   +  4.86E-12 * SQRT(ZPC(2))
     1         +  5.93E-10 * SQRT(ZPC(3)))**2/(FG(4,2) * WN(4,2)**2)
      FG(4,3)=( 7.40E-2  * ZPN(2)   +  6.34E-2 * ZPN(3))/WN(4,3)
      GP(4,3)=(8.22E-12 * SQRT(ZPN(2))   +  7.50E-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))
     1         /WN(5,2)
      GP(5,2)=(3.65E-11 * SQRT(ZPC(1))   +  5.77E-10 * SQRT(ZPC(2))
     1         +  6.56E-11 *  SQRT(ZPC(4)))**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 * ZPO(1)/WN(5,4)
      GP(5,4)=5.08E-12 * 5.08E-12 * ZPO(1)/(FG(5,4) * WN(5,4)**2)
      FMUL(5,L)=FMUC(6,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-2 * 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)=(0.184 * ZPN(1)   +  0.290 * ZPN(2)   +  8.52E-2 * ZPN(3))
     1         /WN(6,3)
      GP(6,3)=(1.07E-11 * SQRT (ZPN(1))   +  4.28E-11 * SQRT(ZPN(2))
     1         +  2.09E-10 * SQRT(ZPN(3)))**2/(FG(6,3) * WN(6,3)**2)
      FG(6,4)=(.120 * ZPO(2)   +  0.151 * ZPO(3))/WN(6,4)
      GP(6,4)=(8.85E-12 * SQRT(ZPO(2))   +  9.93E-12 * SQRT(ZPO( 3)))**2
     1         /(FG(6,4) * WN(6,4)**2)
      FMUL(6,L)=FMUC(7,L)
C   GROUP  7
      FG(7,2)=(4.51E-2 * ZPC(1)   +  0.765 * ZPC(2))/WN(7,2)
      GP(7,2)=(6.07E-10 * SQRT(ZPC(1))   +  2.10E-10 * SQRT(ZPC(2)))**2
     1         /(FG(7,2) * WN(7,2)**2)
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```
      FG(7,3)=(0.454 * ZPN(1)  +  9.66E-2 * ZPN(2)                      TRAN2890
     1        +  0.178 * ZPN(3))/WN(7,3)                                 TRAN2900
      GP(7,3)=(2.71E-12 * SQRT(ZPN(1))  +  2.34E-10 * SQRT(ZPN(2))      TRAN2910
     1        +  2.46E-11 * SQRT(ZPN(3)))**2/(FG(7,3)* WN(7,3)**2)      TRAN2920
      FG(7,4)=4.23E-2 * ZPO(3)/WN(7,4)                                   TRAN2930
      GP(7,4)=2.52E-11 * 2.52E-11 * ZPO(3)/(FG(7,4) * WN(7,4)**2)       TRAN2940
      FMUL(7,L)=FMUC(9,L)                                                TRAN2950
C   GROUP  8                                                             TRAN2960
      FG(8,1)=0.108 * ZPH(1)/WN(8,1)                                     TRAN2970
      GP(8,1)=1.32E-10  *  1.32E-10 * ZPH(1)                             TRAN2980
     1        /(FG(8,1) * WN(8,1)**2)                                    TRAN2990
      FG(8,2)=(0.379 * ZPC(1)  +  1.05 * ZPC(3))/WN(8,2)                 TRAN3000
      GP(8,2)=(1.95E-11 * SQRT(ZPC(1))  +  1.27E-10 * SQRT(ZPC(3)))**2  TRAN3010
     1        /(FG(8,2) * WN(8,2)**2)                                    TRAN3020
      FG(8,3)=(0.155 * ZPN(1)  +  0.142*ZPN(2)  +  3.75E-2 * ZPN(3))    TRAN3030
     1        /WN(8,3)                                                   TRAN3040
      GP(8,3)=(2.98E-11 * SQRT(ZPN(1))  +  7.08E-11 * SQRT(ZPN(2))      TRAN3050
     1        +  1.33E-10 * SQRT(ZPN(3)))**2/(FG(8,3) * WN(8,3)**2)     TRAN3060
      FG(8,4)=(0.146 * ZPO(1)  +  8.61E-2*ZPO(2)                         TRAN3070
     1        +  9.33E-2 * ZPO(3))/WN(8,4)                               TRAN3080
      GP(8,4)=(1.97E-10 * SQRT(ZPO(1))  +  1.80E-11 * SQRT(ZPO(2))      TRAN3090
     1        +  8.13E-11 * SQRT(ZPO(3)))**2/(FG(8,4) * WN(8,4)**2)     TRAN3100
      FMUL(8,L)=FMUC(10,L)                                               TRAN3110
C   GROUP  9                                                             TRAN3120
      FG(9,2)=2.95 * ZPC(2)/WN(9,2)                                      TRAN3130
      GP(9,2)=5.85E-12 * 5.85E-12 * ZPC(2)/(FG(9,2) * WN(9,2)**2)       TRAN3140
      FG(9,3)=(0.224 * ZPN(1)  +  2.92E-2 * ZPN(2))/WN(9,3)             TRAN3150
      GP(9,3)=(3.41E-10 * SQRT(ZPN(1))  +  1.48E-10 * SQRT(ZPN(2)))**2  TRAN3160
     1        /(FG(9,3) * WN(9,3)**2)                                    TRAN3170
      FG(9,4)=(5.24E-2 * ZPO(1)  +  7.22E-2 * ZPO(2)                     TRAN3180
     1        +  6.04E-2 * ZPO(3))/WN(9,4)                               TRAN3190
      GP(9,4)=(5.76E-12 * SQRT(ZPO(1))  +  7.20E-11 * SQRT(ZPO(2))      TRAN3200
     1        +  8.05E-11 * SQRT(ZPO(3)))**2/(FG(9,4) * WN(9,4)**2)     TRAN3210
      FMUL(9,L)=FMUC(11,L)                                               TRAN3220
C                                                                        TRAN3230
C **   PLANCK FUNCTION  **                                               TRAN3240
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C                                                                       TRAN3250
      DO 9 J=1,NHVL                                                     TRAN3260
      BEEL(J,L)=5.04E3 * HVJ(J)**3 / (EXP(HVJ(J)/T1)  -  1.0)          TRAN3270
C                                                                       TRAN3280
C **   INDUCED EMISSION FACTOR (EQ 81)   **                             TRAN3290
C                                                                       TRAN3300
      SSM(J,1,L)=1.10E-16*SNDH (L)*(1.0-EXP(-HVJ(J)/T1)) * FG(J,1)      TRAN3310
      SSM(J,2,L)=1.10E-16*SNDC (L)*(1.0-EXP(-HVJ(J)/T1)) * FG(J,2)      TRAN3320
      SSM(J,3,L)=1.10E-16*SNDN (L)*(1.0-EXP(-HVJ(J)/T1)) * FG(J,3)      TRAN3330
      SSM(J,4,L)=1.10E-16*SNDO (L)*(1.0-EXP(-HVJ(J)/T1)) * FG(J,4)      TRAN3340
      DO 10 M=1,4                                                       TRAN3350
      GGM(J,M,L)=GP(J,M) * SNDE(L)   * (T(L)/1.0E4)**0.25               TRAN3360
     1          +  1.0E-6                                               TRAN3370
      IF(L.GT.1) GO TO 11                                               TRAN3380
      ETAM(J,M,1)=0.                                                    TRAN3390
      SBM (J,M,1)=0.                                                    TRAN3400
      GO TO 10                                                          TRAN3410
   11 ETAM(J,M,L)=ETAM(J,M,L-1)+  (YD(L)-YD(L-1))                       TRAN3420
     1          *(SSM(J,M,L-1) * GGM(J,M,L-1)  +  SSM(J,M,L) * GGM(J,M,L))TRAN3430
     2          * DELTA/3.14159265                                      TRAN3440
      SBM(J,M,L)=SBM(J,M,L-1)  +  (YD(L)-YD(L-1))                       TRAN3450
     1          * (SSM(J,M,L-1)+SSM(J,M,L)) * DELTA                     TRAN3460
   10 CONTINUE                                                          TRAN3470
      IF (L.GT.1) GO TO 12                                              TRAN3480
      TAUL(J,1)=0.                                                      TRAN3490
      GO TO 9                                                           TRAN3500
   12 TAUL(J,L)=TAUL(J,L-1)  +  (YD(L)-YD(L-1))                         TRAN3510
     1          * (FMUL(J,L-1)+FMUL(J,L))  * DELTA                      TRAN3520
    9 CONTINUE                                                          TRAN3530
      IF (IDG.NE.99) GO TO 91                                           TRAN3540
      CALL BUGPR (7)                                                    TRAN3550
C                                                                       TRAN3560
   91 CONTINUE                                                          TRAN3570
      IEZ=IEZ+1                                                         TRAN3580
      ETZ(IEZ)=1.0                                                      TRAN3590
C                                                                       TRAN3600
```

```
C **   CONTINUUM - CONTINUUM FLUX DIVERGENCE CALCULATION  **
C
      DO 300 K=1,IEZ
      DO 31 LK=1,NES
      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
      QCLP(J)=0.
      QLCP(J)=0.
      QLLP(J)=0.
      DO 1612 L=1,NES
      FM(J,L)=0.
 1612 FP(J,L)=0.
      DO 1613 L=1,IEZ
      QCL(L)=0.
      QLC(L)=0.
 1613 QLL(L)=0.
      DO 49 IYY=1,IEZ
      IY=NUT(IYY)
      DO 20 K=1,12
      FMC(K,IY)=0.
      FPC(K,IY)=0.
      IF (IY.EQ.1) GO TO 44
      DO 40 L=1,IY
C
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
C **    MINUS CONTINUUM FLUX (EQ 46)  **
C
      FMC(K,IY)=FMC(K,IY)  -  (EM(K,L)-EM(K,L-1))
```

```
     1          * (BEEC(K,L-1)+BEEC(K,L))/2.                                   TRAN3970
   43 CONTINUE                                                                 TRAN3980
   44 IF (IY.EQ.NES ) GO TO 41                                                 TRAN3990
      DO 42 L=IY,NES                                                           TRAN4000
C                                                                              TRAN4010
C **   POSITIVE EMISSIVITY FUNCTION (EQ 47)  **                                TRAN4020
C                                                                              TRAN4030
      EP(K,L)=1.0   -  EXP(TAUC(K,IY)-TAUC(K,L))                               TRAN4040
      IF (L.EQ.IY) GO TO 42                                                    TRAN4050
C                                                                              TRAN4060
C **   POSITIVE EMISSIVITY CONTINUUM FLUX (EQ 46)  **                          TRAN4070
C                                                                              TRAN4080
      FPC(K,IY)=FPC(K,IY)  +  (EP(K,L)-EP(K,L-1))                              TRAN4090
     1          * (BEEC(K,L-1)+BEEC(K,L))/2.                                   TRAN4100
   42 CONTINUE                                                                 TRAN4110
C                                                                              TRAN4120
C **   POSITIVE EMISSIVITY CONTINUUM FLUXDIVERGENCE (EQ 51)  **                TRAN4130
C                                                                              TRAN4140
   41 QCCP(K)=6.2831853 * FMUC(K,IY) *                                         TRAN4150
     1          (FMC(K,IY)  +  FPC(K,IY)  -  2.0* BEEC(K,IY))                  TRAN4160
      FMC(K,IY)=FMC(K,IY) * 3.14159265                                         TRAN4170
      FPC(K,IY)=FPC(K,IY) * 3.14159265                                         TRAN4180
   20 CONTINUE                                                                 TRAN4190
C                                                                              TRAN4200
C **   DEBUG PRINT  **                                                         TRAN4210
C                                                                              TRAN4220
      IF (IDG.NE.99) GO TO 21                                                  TRAN4230
      CALL BUGPR (3)                                                           TRAN4240
   21 QCC(IYY)=0.                                                              TRAN4250
      DO 24 K=1,12                                                             TRAN4260
C                                                                              TRAN4270
C **   LINE AND CROSS TERM FLUX DIVERGENCE CALCULATION  **                     TRAN4280
C                                                                              TRAN4290
   24 QCC(IYY)=QCC(IYY)   +  QCCP(K)                                           TRAN4300
      IF (LINES.EQ.0) GO TO 1614                                               TRAN4310
C                                                                              TRAN4320
```

```
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.IY) 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 RRM=DIF/2.0/GGM(J,M,IY)**2
      WWM=6.2831853 * WN(J,M) * BETAM * GAMMA(TM) * TM
      SUM1=SUM1  +  GAMMA(TM) * WN(J,M) * SSM(J,M,IY)
      SUM2=SUM2  +  XLAMB(RRM) * WN(J,M) * SSM(J,M,IY)
   67 WIM=WIM  +  WWM
      ALPHAM=WIM/DJ(J)
C
C **   OVERLAPPING LINE CALCULATIONS  **
C
C
C **   GROUP EQUIVALENT WIDTHS  (EQ.88)  **
C
      WMM(J,L)=DJ(J) * PHI1(ALPHAM) * EXP(TAUL(J,L)-TAUL(J,IY))
C
C **   GROUP GAMMA -- LINE TRANSPORT FUNCTION (EQ.92)  **
C
      GMM(J,L)=PHI2(ALPHAM) * SUM1
```

```
C                                                                       TRAN4690
C **   MINUS EMISSIVITY FUNCTION FOR LINES (EQ.47)   **                 TRAN4700
C                                                                       TRAN4710
      EEM(J,L)=1.0  -  EXP(TAUL(J,L)-TAUL(J,IY))                        TRAN4720
   66 XLMM(J,L)=PHI2(ALPHAM) * SUM2                                     TRAN4730
   65 CONTINUE                                                          TRAN4740
      IF (IDG.EQ.99) CALL BUGPR(1)                                      TRAN4750
      IF (IDG.EQ.99) CALL BUGPR (4)                                     TRAN4760
   68 IF (IY.EQ.NES) GO TO 72                                           TRAN4770
C                                                                       TRAN4780
C **   INTEGRATION FROM IY TO NES   **                                  TRAN4790
C                                                                       TRAN4800
      DO 69 J=1,9                                                       TRAN4810
      DO 70 L=IY,NES                                                    TRAN4820
      WIP=0.                                                            TRAN4830
      SUM1=0.                                                           TRAN4840
      SUM2=0.                                                           TRAN4850
      DO 71 M=1,4                                                       TRAN4860
      DIF=ETAM(J,M,L)  -  ETAM(J,M,IY)                                  TRAN4870
      DIFSBM =     SBM(J,M,L)-SBM(J,M,IY)                               TRAN4880
      IF(ABS(DIFSBM).LT.1.E-10)  DIFSBM = 1.E-10                        TRAN4890
      BETAP=DIF / ( DIFSBM                 )  *  3.14159265             TRAN4900
      IF (L.EQ.IY) BETAP=GGM(J,M,L)                                     TRAN4910
      IF(ABS(DIF).GT.1.E-10) GO TO 9003                                 TRAN4920
      TP  =  1.E-10                                                     TRAN4930
      GO TO 9004                                                        TRAN4940
 9003 CONTINUE                                                          TRAN4950
      TP=DIF/2.0/BETAP**2                                               TRAN4960
 9004 RRP=DIF/2.0/GGM(J,M,IY)**2                                        TRAN4970
      WWP=6.2831853 * WN(J,M) * BETAP * GAMMA(TP) * TP                  TRAN4980
      SUM1=SUM1  +  GAMMA(TP) * WN(J,M) * SSM(J,M,IY)                   TRAN4990
      SUM2=SUM2  +  XLAMB(RRP) * WN(J,M) * SSM(J,M,IY)                  TRAN5000
   71 WIP=WIP+WWP                                                       TRAN5010
      ALPHAP=WIP/DJ(J)                                                  TRAN5020
      WPP(J,L)=DJ(J) * PHI1(ALPHAP) * EXP(TAUL(J,IY)-TAUL(J,L))         TRAN5030
      GPP(J,L)=PHI2(ALPHAP) * SUM1                                      TRAN5040
```

```
C                                                                       TRAN5050
C **   POSITIVE EMISSIVITY FUNCTION FOR LINES (EQ.47)  **               TRAN5060
C                                                                       TRAN5070
      EEP(J,L)=1.0  -  EXP(TAUL(J,IY)-TAUL(J,L))                        TRAN5080
   70 XLPP(J,L)=PHI2(ALPHAP) * SUM2                                     TRAN5090
   69 CONTINUE                                                          TRAN5100
C                                                                       TRAN5110
C **   DEBUG PRINT  **                                                  TRAN5120
      IF (IDG.EQ.99) CALL BUGPR (5)                                     TRAN5130
C                                                                       TRAN5140
   72 DO 80 J=1,9                                                       TRAN5150
      ASM1=0.                                                           TRAN5160
      ASM2=0.                                                           TRAN5170
      FM(J,IY)=0.                                                       TRAN5180
      IF (IY.EQ.1) GO TO 81                                             TRAN5190
      DO 82 L=2,IY                                                      TRAN5200
      FM(J,IY)=FM(J,IY)  -  (WMM(J,L)-WMM(J,L-1))                       TRAN5210
     1       *(BEEL(J,L-1)+BEEL(J,L)) * 1.5707963                       TRAN5220
      IF (L.EQ.IY) GO TO 82                                             TRAN5230
      ASM1=ASM1  -  (EEM(J,L)-EEM(J,L-1))                               TRAN5240
     1        * (BEEL(J,L-1) * XLMM(J,L-1) + BEEL(J,L) * XLMM(J,L))/2.  TRAN5250
      ASM2=ASM2  -  (XLMM(J,L)-XLMM(J,L-1))                             TRAN5260
     1        * (BEEL(J,L-1) * EXP(TAUL(J,L-1)-TAUL(J,IY)) + BEEL(J,L)  TRAN5270
     2        * EXP(TAUL(J,L)-TAUL(J,IY)))/2.0                          TRAN5280
   82 CONTINUE                                                          TRAN5290
   81 ASP1=0.                                                           TRAN5300
      ASP2=0.                                                           TRAN5310
      IYP=IY+1                                                          TRAN5320
      IF (IY.EQ.NES) GO TO 83                                           TRAN5330
      DO 84 L=IYP,NES                                                   TRAN5340
      FP(J,IY)=FP(J,IY)  +  (WPP(J,L)-WPP(J,L-1))                       TRAN5350
     1        * (BEEL(J,L-1)+BEEL(J,L)) * 1.5707963                     TRAN5360
      IF (L.EQ.IYP) GO TO 84                                            TRAN5370
      ASP1=ASP1  +  (EEP(J,L)-EEP(J,L-1))                               TRAN5380
     1        * (BEEL(J,L-1) * XLPP(J,L-1) + BEEL(J,L) * XLPP(J,L))/2.0 TRAN5390
      ASP2=ASP2  +  (XLPP(J,L)-XLPP(J,L-1)) *                           TRAN5400
```

```
     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.
     DO 86 M=1,4
  86 SUMT=SUMT  +  SSM(J,M,IY) * WN(J,M)
     ATM1=0.
     IF (IY.NE.1) ATM1=(BEEL(J,IY-1)+BEEL(J,IY)) /2.0 * EEM(J,IY-1)
    1           * XLMM(J,IY-1)
     ATP1=0.
     IF(IY.NE.NES) ATP1=(BEEL(J,IY+1)+BEEL(J,IY))/2.0 * EEP(J,IY+1)
    1           * XLPP(J,IY+1)
     QCLP(J)=6.2831853  * SUMS * (ASM1+ASP1+ATM1+ATP1)
     IF (IY.EQ.1) ATM2=-BEEL(J,IY) * SUMT
     IF (IY.NE.1) ATM2=(BEEL(J,IY-1)-BEEL(J,IY))  *  GMM(J,IY-1)
    1           -  BEEL(J,IY-1) * XLMM(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           -  BEEL(J,IY+1) * XLPP(J,IY+1)
     QLLP(J)=6.2831853 * 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)
  85 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
      DQ(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=0.0
      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
C
C **  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  SND(I)
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(50),C (20,60),EC(5,60)
      COMMON /REFLUX/ E(60),IRAD,ITYPE
      COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON/WT/SMW(20),AWT(5)
      COMMON /NUMDEN/ SNDO2(60), SNDN2(60), SNDO(60), SNDN(60),
     1                                      SNDE(60), SNDC(60),
     2                 SNDH(60), SNDC2(60), SNDH2(60), SNDCO(60),
     3                 SNDC3(60),SNDC2H(60)
C     **  CALCULATE SPECIE NUMBER DENSITIES BASED ON MOLE FRACTIONS  **
C
      CONVER = 3.10375E+23 *RHO(I) *RDZ
C
      SNDO2(I) = CONVER * C( 1,I)/SMW( 1)
      SNDN2(I) = CONVER * C( 2,I)/SMW( 2)
      SNDO (I) = CONVER * C( 3,I)/SMW( 3)
      SNDN (I) = CONVER * C( 4,I)/SMW( 4)
      SNDE (I) = CONVER * C( 7,I)/SMW( 7)
      SNDC (I) = CONVER * C( 8,I)/SMW( 8)
      SNDH (I) = CONVER * C( 9,I)/SMW( 9)
      SNDH2(I) = CONVER * C(10,I)/SMW(10)
      SNDCO(I) = CONVER * C(11,I)/SMW(11)
      SNDC3(I) = CONVER * C(12,I)/SMW(12)
      SNDC2(I) = CONVER * C(19,I)/SMW(19)
      SNDC2H(I)= CONVER * C(14,I)/SMW(14)
      RETURN
      END
```

```
      SUBROUTINE LRAD
C
C
C  **  THIS IS A DRIVER PROGRAM FOR SUBROUTINE TRANS WHICH CALCULATES **
C      THE RADIATIVE FLUX DIVERGENCE THROUGH A ONE-DIMENSIONAL SLAB
C      FOR A GIVEN TEMPERATURE AND SPECIES DISTRIBUTION
      COMMON /SFLUX/ QRI(3)
      COMMON /TRN/          NUT(60), FMC(12,60), FPC(12,60),
     1              FM(9,60), FP(9,60), LINES
      COMMON /TEST/ETZ(60),IEZ
      COMMON /YL/ETA(60),YOND(60)
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(60),C (20,60),EC(5,60)
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /NON/RDZ,MUDZ,RMDZ,AKNF,HNF,CPNF
      COMMON /MAIM/KEEP,MAXE,MAXM,MAXD,    IDG,MCONV,ECONV,DCONV,LT,IAB
      COMMON /RFLUX/ E(60),IRAD,ITYPE
      COMMON /NUMDEN/ SNDO2(60), SNDN2(60), SNDO(60), SNDN(60),
     1                                      SNDE(60), SNDC(60),
     2                SNDH(60), SNDC2(60), SNDH2(60), SNDCO(60),
     3                SNDC3(60),SNDC2H(60)
      COMMON /SPEC/ MF, XMOL
C
C
C  **  NETA = NUMBER OF ETA POINTS
C      MF   = 1  IF SPECIE  MOLE FRACTIONS ARE INPUT AND NUMBER DENSITY
C                TO BE COMPUTED
C              0 IF SPECIE NUMBER DENSITIES ARE INPUT
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
C
```

```
C   **  R        = BODY RADIUS (FT)
C       DELTA    = NONDIMENSIONAL STAND-OFF DISTANCE
C       DTIL     = TRANSFORMED STAND-OFF DISTANCE
C       XMOL     = 1.C FOR RUN WITH MOLECULES
C                  C.C FOR RUN WITHOUT MOLECULES
C
      XMOL  = 0.0
      XMOL= 1.0
C
C     ** DETERMINE ETZ POINTS
      N2 = NETA-2
      K =0
      IEZ =0
      DO 20 I=1,N2,2
      K=K+1
 20   ETZ(K) = ETA(I)
      ETZ(K+1) = ETA(NETA-1)
      ETZ(K+2) = ETA(NETA)
      IEZ = K +1
C
C     **  COMPUTE THE  Y  COORDINATE   **
      YOND(1) = 0.0
      SUM = 0.0
      DO 30 K=2,NETA
      DETA = ETA(K) -ETA(K-1)
      SUM = SUM +DETA*(1./RHO(K) +1./RHO(K-1) )/2.C
      YOND(K) = DTIL *SUM
 30   CONTINUE
      DELTA = YOND(NETA)
      DO 40 K=1,NETA
      YOND(K) = YOND(K)/YOND(NETA)
 40   CONTINUE
C
      LINES= 1
      IDG3 = IDG
      IDG = 0
```

```
      CALL TRANS(1)                                                      LRAD 730
      IDG= IDGS                                                          LRAD 740
C                                                                        LRAD 750
C  **  INDEX IS NUMBER GIVEN SPECIE FOR USE IN STORING ARRAYS **         LRAD 760
C                        1      =     O2                                 LRAD 770
C                        2      =     N2                                 LRAD 780
C                        3      =     O                                  LRAD 790
C                        4      =     N                                  LRAD 800
C                        5      =     E-                                 LRAD 810
C                        6      =     C                                  LRAD 820
C                        7      =     H                                  LRAD 830
C                        8      =     C2                                 LRAD 840
C                        9      =     H2                                 LRAD 850
C                       10      =     CO                                 LRAD 860
C                       11      =     C3                                 LRAD 870
C                       12      =     C2H                                LRAD 880
C                                                                        LRAD 890
C                                                                        LRAD 900
      RETURN                                                             LRAD 910
      END                                                                LRAD 920
```

```
      SUBROUTINE ZP(T1,SUMN,SUMO,SUMH,SUMC)
C
C     **  FRACTIONAL POPULATION STATES FOR N, O, H, C   **
C
      COMMON /ZPI/ ZPO(6), ZPN(6),ZPH(2),  ZPC(7)
      ZPH(1)=2.0/SUMH
      ZPH(2)=8.0 * EXP(-10.20/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
C
      RETURN
      END
```

```
      SUBROUTINE TRANS2
      COMMON /SFLUX/ QRI(3)
      COMMON /YL/ETA(60),YOND(60)
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, 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/ETZ(60),IEZ
      COMMON /NUMDEN/ SNDO2(60), SNDN2(60), SNDO(60), SNDN(60),
     1                                       SNDE(60), SNDC(60),
     2                SNDH(60), SNDC2(60), SNDH2(60), SNDCO(60),
     3                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),SNDN2(I),SNDO2(I),SNDN(I),SNDO(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 (6,4103)
      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
```

```
      L1=NUT(1)                                                         TRAN 370
      L2=NUT(2)                                                         TRAN 380
      L3=NUT(3)                                                         TRAN 390
      WRITE (6,8037)(ETOUT(IL),IL=1,3)                                  TRAN 400
      FM1=0.0                                                           TRAN 410
      FP1=0.0                                                           TRAN 420
      FM2=0.0                                                           TRAN 430
      FP2=0.0                                                           TRAN 440
      FM3=0.0                                                           TRAN 450
      FP3=0.0                                                           TRAN 460
      DO 4104 KL=1,NIHVC                                                TRAN 470
      WRITE (6,8042) KL,   FHVC(KL),   FMC(KL,L1),   FPC(KL,L1),        TRAN 480
     1              FMC(KL,L2),   FPC(KL,L2),  FMC(KL,L3),   FPC(KL,L3) TRAN 490
      FM1=FM1  +  FMC(KL,L1)                                            TRAN 500
      FP1=FP1  +  FPC(KL,L1)                                            TRAN 510
      FM2=FM2  +  FMC(KL,L2)                                            TRAN 520
      FP2=FP2  +  FPC(KL,L2)                                            TRAN 530
      FM3=FM3  +  FMC(KL,L3)                                            TRAN 540
      FP3=FP3  +  FPC(KL,L3)                                            TRAN 550
 4104 CONTINUE                                                          TRAN 560
      WRITE (6,8045) FM1,   FP1,   FM2,   FP2,   FM3,   FP3             TRAN 570
      QRI(1)=FM1+FP1                                                    TRAN 580
      QRI(2)=FM2+FP2                                                    TRAN 590
      QRI(3)=FM3+FP3                                                    TRAN 600
C                                                                       TRAN 610
C **   LINE       CONTRIBUTION TO THE SPECTRAL FLUX **                  TRAN 620
C                                                                       TRAN 630
      IF (LINES.EQ.0) RETURN                                            TRAN 640
      WRITE (6,8035)                                                    TRAN 650
      WRITE (6,8037) (ETOUT(IL),IL=1,3)                                 TRAN 660
      FM1=0.0                                                           TRAN 670
      FP1=0.0                                                           TRAN 680
      FM2=0.0                                                           TRAN 690
      FP2=0.0                                                           TRAN 700
      FM3=0.0                                                           TRAN 710
      FP3=0.0                                                           TRAN 720
```

```
C
C **   TOTAL FLUX CALCULATION   **
C
      DO 8043 KL=1,NHVL
      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)
 8043 CONTINUE
      WRITE (6,8045) FM1,   FP1,   FM2,   FP2,   FM3,   FP3
      QRI(1)=QRI(1)  +  FM1  +  FP1
      QRI(2)=QRI(2)  +  FM2  +  FP2
      QRI(3)=QRI(3)  +  FM3  +  FP3
C
  600 FORMAT (1H1,33HNUMBER DENSITIES  (PARTICLES/CM3) ///5X,3HETA, 8X,
     1          2HN2, 8X,2HO2, 8X,1HN, 8X,1HO, 9X, 2HE-,8X,
     2 1HH,8X,1HC, 8X,2HC2, 8X,2HH2, 8X,2HCO, 8X,2HC3,8X,3HC2H///)
  603 FORMAT (1P13E10.2)
 4103 FORMAT (44H1CONTINUUM CONTRIBUTION TO THE SPECTRAL FLUX)
 8035 FORMAT (39H0LINE CONTRIBUTION TO THE SPECTRAL FLUX)
 8037 FORMAT (/22X,5HETA =F7.3,13X,5HETA =F7.3,13X,5HETA =F7.3//3X,1HI,
     1 3X,3HHNU,8X,6HQMINUS,7X,5HQPLUS,8X,6HQMINUS,7X,5HQPLUS,8X,
     2 6HQMINUS,7X,5HQPLUS/)
 8042 FORMAT (I4,F8.3,1P8E13.3)
 8045 FORMAT (12H0TOTAL FLUX ,1P8E13.3)
      RETURN
      END
```

```
      SUBROUTINE BUGPR (IDGSW)                                          BUGP  10
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NES    BUGP  20
      COMMON /YL/ETA(60),  YD(60)                                       BUGP  30
      COMMON /TRN/       NUT(60), FMC(12,60), FPC(12,60),               BUGP  40
     1              FM(9,60),  FP(9,60), LINES                          BUGP  50
      COMMON /DBUG/ QLC(60), QCL(60), QLL(60), DQN(60), QCC(60),        BUGP  60
     1              BEEC(12,60),    FMUC(12,60),    EM(12,60),          BUGP  70
     2              EP(12,60),      TAUC(12,60),    BEEL(9,60),         BUGP  80
     3              QCCP(12),       WMM(9,60),      GMM(9,60),          BUGP  90
     4              EEM(9,60),      XLMM(9,60),     QLCP(9),            BUGP 100
     5              QCLP(9),        QLLP(9),        DELTA,    IY,  IYY, BUGP 110
     6              WPP(9,60),      GPP(9,60),      EEP(9,60),          BUGP 120
     7              XLPP(9,60),     FG(9,4),        GP(9,4),            BUGP 130
     8              WN(9,4),        FMUL(9,60),     SSM(9,4,60),        BUGP 140
     9              GGM(9,4,60),    ETAM(9,4,60),   SBM(9,4,60),        BUGP 150
     A              TAUL(9,60)                                          BUGP 160
      GO TO (10,20,30,40,50,60,70), IDGSW                               BUGP 170
   10               WRITE (6,194)                                       BUGP 180
  194 FORMAT (1H1)                                                      BUGP 190
      RETURN                                                            BUGP 200
   20 WRITE (6,7182) DELTA                                              BUGP 210
 7182 FORMAT (7H0DELTA=1PE14.7,3H CM)                                   BUGP 220
      RETURN                                                            BUGP 230
   30 WRITE (6,190) IY,    YD(IY)                                       BUGP 240
  190 FORMAT (4H1 IY=I3,2X,3HYD=1PE12.5//2X,1HK,2X,1HL,7X,3HETA,13X,2HYD,BUGP 250
     1 13X,2HMU,11X,3HTAU,14X,1HE,11X,3HBEE//)                          BUGP 260
      DO 22 K=1,12                                                      BUGP 270
      IF (IY.EQ.1) GO TO 23                                             BUGP 280
      WRITE(6,191) (K,   L,    ETA(L),   YD(L),   FMUC(K,L),   TAUC(K,L),BUGP 290
     1             FM(K,L),   BEEC(K,L),   L=1,IY)                      BUGP 300
  191 FORMAT (2I3,1P6E15.5)                                             BUGP 310
      WRITE (6,192)                                                     BUGP 320
  192 FORMAT (//)                                                       BUGP 330
   23 IF (IY.EQ.NES) GO TO 22                                           BUGP 340
      WRITE (6,191) (K,   L,   ETA(L),   YD(L),   FMUC(K,L),            BUGP 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)                       BUGP 370
193 FORMAT (5H0FIM=1PE12.5 ,2X,4HFIP=E12.5,2X,5HQCCP=E12.5)                  BUGP 380
    RETURN                                                                  BUGP 390
40                  WRITE (6,195) IY,   YD(IY),    ((J,    L,    YD(L),     BUGP 400
   1              WMM(J,L),    GMM(J,L),    XLMM(J,L),    EEM(J,L),         BUGP 410
   2              BEEL(J,L),    L=1,IY),    J=1,9)                          BUGP 420
195 FORMAT (4H0IY=I3,2X,3HYY=1PE12.5//2X,1HJ,2X,1HL,7X,2HYD,12X,3HWMM,BUGP 430
   1 12X,3HGMM,11X,4HXLMM,13X,3HEEM,13X,3HBEE//(2I3,6E16.5))                BUGP 440
    RETURN                                                                  BUGP 450
50                  WRITE (6,196) IY,   YD(IY),    ((J,    L,    YD(L),     BUGP 460
   1          WPP(J,L),    GPP(J,L),    XLPP(J,L),    EEP(J,L),             BUGP 470
   2          BEEL(J,L),    L=IY,NES),    J=1,9)                            BUGP 480
196 FORMAT (4H0IY=I3,2X,3HYY=1PE12.5//2X,1HJ,2X,1HL,7X,2HYD,13X,3HWPP,BUGP 490
   1 2X,3HGPP,11X,4HXLPP,13X,3HEEP,13X,3HBEE//(2I3,6E16.5))                 BUGP 500
    RETURN                                                                  BUGP 510
60  WRITE (6,198) IY,    ETA(IY),    YD(IY)                                 BUGP 520
198 FORMAT (4H0IY=I3,2X,4HETA=1PE12.5,2X,3HYY=E12.5//2X,1HJ,5X,3HQCC,  BUGP 530
   1 11X,3HFMC,11X,3HFPC,11X,3HQCL,11X,3HQLC,11X,3HQLL,12X,2HFM,12X,        BUGP 540
   2 2HFP,11X,3HDQN//)                                                      BUGP 550
    WRITE (6,199) (J,    QCCP(J),    FMC(J,IY),    FPC(J,IY),               BUGP 560
   1              QCLP(J),    QLCP(J),    QLLP(J),    FM(J,IY),FP(J,IY),    BUGP 570
   2              J=1,9)                                                    BUGP 580
199 FORMAT (I3,1P8E14.5)                                                    BUGP 590
    WRITE (6,8069) (J,    QCCP(J),    FMC(J,IY),    FPC(J,IY),    J=10,12)BUGP 600
8069 FORMAT (I3,1P3E14.5)                                                   BUGP 610
    WRITE (6,200) QCC(IYY),    QCL(IYY),    QLC(IYY),    QLL(IYY),          BUGP 620
   1              DQN(IYY)                                                  BUGP 630
200 FORMAT (1H0,2X,1PE14.5,28X,3E14.5,28X,E14.5)                            BUGP 640
    RETURN                                                                  BUGP 650
70  WRITE (6,197) L,    ETA(L),    YD(L),    ((J,    M,    WN(J,M),         BUGP 660
   1              FG(J,M),    GP(J,M),    FMUL(J,L),    TAUL(J,L),          BUGP 670
   2              SSM(J,M,L),    GGM(J,M,L),    ETAM(J,M,L),    SBM(J,M,L),BUGP 680
   3              M=1,4),J=1,9)                                             BUGP 690
197 FORMAT (3H0L=I3,2X,4HETA=1PE12.5,2X,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//(2I3,9E14.5))                                        BUGP 720
```

```
RETURN                                                    BUGP 730
END                                                       BUGP 740
```

```
      SUBROUTINE ZHV(HV,ZO,ZN,ZI,ZC)
C
C
C  ** THIS SUBROUTINE CALCULATES THE QUANTUM MECHANICAL CORRECTION
C          FACTORS GIVEN A FREQUENCY (HV) **
C
      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 ZO = .9999795             -.3155480*X           +2.824548 E-02*X2
     1     +6.677328 E-03*X3    -3.644585 E-03*X4     +8.058070 E-04*X5
     2     -7.708637 E-05*X6    +2.668133 E-06*X7
      GO TO 3
    2 ZO = (X/9.82)**3
    3 IF (X -8.35) 4,4,5
    4 ZN = 1.000148             - .4183535 *X         + .1680359 *X2
     1     -9.779458 E-02*X3    +3.354635 E-02*X4     -5.609353 E-03*X5
     2     +4.515535E-04*X6     -1.403585 E-05*X7
      GO TO 6
    5 ZN = (X/8.35)**3
    6 Y = X/4.0
      IF (Y-6.6) 9,9,10
    9 Y2 =Y*Y
      Y3 =Y2*Y
      Y4 =Y3*Y
      Y5 =Y4*Y
      Y6 =Y5*Y
      Y7 =Y6*Y
      ZI = 1.000379             - .2364767 *Y         +7.505242 E-02*Y2
     1     -1.702948E-02*Y3     +3.279554 E-03*Y4     -2.128469 E-04*Y5
      GO TO 11
```

```
10    ZI = (Y/6.6)**3                                                                        ZHV( 370
11    IF (X-7.37) 12,12,13                                                                   ZHV( 380
12    ZC =   .9974367           - .4341812 *X           +8.531314 E-02*X2                   ZHV( 390
     1    -1.393917 E-02*X3    +4.038545 E-03*X4      -5.426425 E-04*X5                   ZHV( 400
     2    +2.812126 E-05*X6    -3.883530 E-07*X7                                           ZHV( 410
      GO TO 14                                                                               ZHV( 420
13    ZC = (X/7.37)**3                                                                       ZHV( 430
14    RETURN                                                                                 ZHV( 440
      END                                                                                    ZHV( 450
```

```
      SUBROUTINE RADIN
      COMMON /DHUG/ 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  **
      WN(1,1)=0.
      FG(1,1)=0.
      GP(1,1)=0.
      WN(1,2)=18.
      WN(1,3)=15.
      WN(1,4)=5.
C  **  GROUP 2  **
      WN(2,1)=3.0
      WN(2,2)=5.0
      WN(2,3)=11.0
      WN(2,4)=10.
C  **  GROUP 3  **
      WN(3,1)=0.
      FG(3,1)=0.
      GP(3,1)=0.
      WN(3,2)=2.0
      WN(3,3)=0.
      FG(3,3)=0.
      GP(3,3)=0.
      WN(3,4)=0.
      FG(3,4)=0.
      GP(3,4)=0.
C  **  GROUP 4  **
```

```
      WN(4,1)=0.                                                        RADI 370
      FG(4,1)=0.                                                        RADI 380
      GP(4,1)=0.                                                        RADI 390
      WN(4,2)=8.0                                                       RADI 400
      WN(4,3)=2.0                                                       RADI 410
      WN(4,4)=0.                                                        RADI 420
      FG(4,4)=0.                                                        RADI 430
      GP(4,4)=0.                                                        RADI 440
C   **  GROUP 5   **                                                    RADI 450
      WN(5,1)=0.                                                        RADI 460
      FG(5,1)=0.                                                        RADI 470
      GP(5,1)=0.                                                        RADI 480
      WN(5,2)=14.                                                       RADI 490
      WN(5,3)=4.0                                                       RADI 500
      WN(5,4)=1.0                                                       RADI 510
C   **  GROUP 6   **                                                    RADI 520
      WN(6,1)=1.0                                                       RADI 530
      WN(6,2)=4.0                                                       RADI 540
      WN(6,3)=13.0                                                      RADI 550
      WN(6,4)=2.0                                                       RADI 560
C   **  GROUP 7   **                                                    RADI 570
      WN(7,1)=0.                                                        RADI 580
      FG(7,1)=0.                                                        RADI 590
      GP(7,1)=0.                                                        RADI 600
      WN(7,2)=6.0                                                       RADI 610
      WN(7,3)=14.0                                                      RADI 620
      WN(7,4)=3.0                                                       RADI 630
C   **  GROUP 8   **                                                    RADI 640
      WN(8,1)=2.0                                                       RADI 650
      WN(8,2)=2.0                                                       RADI 660
      WN(8,3)=11.                                                       RADI 670
      WN(8,4)=15.                                                       RADI 680
C   **  GROUP 9   **                                                    RADI 690
      WN(9,1)=0.                                                        RADI 700
      FG(9,1)=0.                                                        RADI 710
      GP(9,1)=0.                                                        RADI 720
```

```
WN(9,2)=1.0
WN(9,3)=11.
WN(9,4)=10.
RETURN
END
```

```
      SUBROUTINE STPSZE
C
C     **  ROUTINE TO ADJUST STEP SIZE AS NEEDED
C         TO MAINTAIN ACCURACY  **
C
C
      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,RZB,PD,HD,HTOTAL
      COMMON /RFLUX/ E(60),IRAD,ITYPE
      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 /OLD/ TOLD(60),EOLD(60),RHOS(60)
C
      N=2
    1 CONTINUE
      I2=2
      IF(NETA.GE. 59) GO TO 5
C
      DO 2 I=N,NETA
      L=I
      CHECK = ABS(G(I)-G(I-1) )
      IF(CHECK .GT. .05) GO TO 3
    2 CONTINUE
C
      GO TO 5
C
    3 CONTINUE
      M = NETA - L + 1
C
      DO 4 I=1,M
      K = NETA - I + 1
```

```
      G(K+1) = G(K)
      F(K+1) =F(K)
      DO100JJ=1,5
100   EC(JJ,K+1)=EC(JJ,K)
      TOLD(K+1)=TOLD(K)
      RHOS(K+1)=RHOS(K)
      RHO(K+1) = RHO(K)
      RM (K+1) = RM (K)
      IF(IRAD.EQ. 3) E(K+1) = E(K)
      ETA(K+1) = ETA(K)
4     CONTINUE
C
      G(L) = (G(L-1) + G(L+1) ) / 2.0
      F(L) = (F(L-1)+F(L+1))/2.
      DO101JJ=1,5
101   EC(JJ,L)=(EC(JJ,L-1)+EC(JJ,L+1))/2.
      TOLD(L)=(TOLD(L-1)+TOLD(L+1))/2.0
      RHOS(L)=(RHOS(L-1)+RHOS(L+1))/2.0
      RHO(L) = (RHO(L-1) +RHO(L+1))/2.
      RM (L) = (RM (L-1) +RM (L+1))/2.
      IF(IRAD.EQ. 3) E(L) =(E(L-1)+ E(L+1))/2.0
      ETA(L) = (ETA(L-1) + ETA(L+1) )/2.0
      NETA = NETA + 1
      N=L
C
      IF( NETA .LT. 59) GO TO 1
C
5     CONTINUE
C
      IF(I2 .GE. NETA) GO TO 10
      DO 6 I=I2,NETA,2
      L=I
      IF (L.EQ.NETA) GO TO 6
      IF(ETA(I).EQ. 0.98) GO TO 6
      CHECK =ABS(G(I+1) - G(I-1) )
      IF(CHECK .LT. 0.005) GO TO 7
```

```
  6   CONTINUE                                                          STPS 730
C                                                                       STPS 740
      GO TO 10                                                          STPS 750
  7   CONTINUE                                                          STPS 760
      I2=L+1                                                            STPS 770
      IF(ETA(L+1)-ETA(L-1).GT. .04) GO TO 5                             STPS 780
C                                                                       STPS 790
      DO 8 I=L,NETA                                                     STPS 800
      G(I) = G(I+1)                                                     STPS 810
      F(I) = F(I+1)                                                     STPS 820
      DO102JJ=1,5                                                       STPS 830
 102  EC(JJ,I)=EC(JJ,I+1)                                               STPS 840
      TOLD(I)=TOLD(I+1)                                                 STPS 850
      RHOS(I)=RHOS(I+1)                                                 STPS 860
      RHO(I) = RHO(I+1)                                                 STPS 870
      RM (I) = RM (I+1)                                                 STPS 880
      IF(IRAD.EQ. 3) E(I) =E(I+1)                                       STPS 890
      ETA(I)=ETA(I+1)                                                   STPS 900
  8   CONTINUE                                                          STPS 910
C                                                                       STPS 920
      NETA=NETA-1                                                       STPS 930
      IF (NETA .GT. 1) GO TO 5                                          STPS 940
C                                                                       STPS 950
 10   CONTINUE                                                          STPS 960
      NN = NETA-2                                                       STPS 970
      DO 20 I=1,NN                                                      STPS 980
      Z(I) = ETA(I+1)/DTIL                                              STPS 990
 20   CONTINUE                                                          STPS1000
      RETURN                                                            STPS1010
      END                                                               STPS1020
```

```
      SUBROUTINE MATINV(A,N,B,M,NMAX)
C
C
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
      DIMENSION A(7,7),B(7,1),IPIVOT(7),INDEX(7,2)
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)
C
C     INITIALIZATION
C
    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)=0
   30 DO 550 I=1,N
C
C     SEARCH FOR PIVOT ELEMENT
C
   40 AMAX=0.0
   45 DO 105 J=1,N
   50 IF (IPIVOT(J)-1)60,105,60
   60 DO 100 K=1,N
   70 IF (IPIVOT(K)-1)80,100,740
   80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100
   85 IROW=J
   90 ICOLUM=K
   95 AMAX=A(J,K)
  100 CONTINUE
  105 CONTINUE
      IF (AMAX)110,106,110
  106 DETERM=0.0
      ISCALE=0
      GO TO 740
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
C
```

```
C        INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
  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
C        SCALE THE DETERMINANT
C
 1000 PIVOTI=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(PIVOTI)-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(ICOLUM,ICOLUM)=1.0
  340 DO 350 L=1,N
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT
  355 IF(M) 380,380,360
  360 DO 370 L=1,M
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT
C
C     REDUCE NON-PIVOT ROWS
C
  380 DO 550 L1=1,N
  390 IF(L1-ICOLUM)400,550,400
  400 T=A(L1,ICOLUM)
  420 A(L1,ICOLUM)=0.0
  430 DO 450 L=1,N
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
  455 IF(M) 550,550,460
  460 DO 500 L=1,M
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
  550 CONTINUE
C
C     INTERCHANGE COLUMNS
  600 DO 710 I=1,N
```

```
C                                                             MATI1090
  610 L=N+1-I                                                 MATI1100
  620 IF(INDEX(L,1)-INDEX(L,2))630,710,630                    MATI1110
  630 JROW=INDEX(L,1)                                         MATI1120
  640 JCOLUM=INDEX(L,2)                                       MATI1130
  650 DO 705 K=1,N                                            MATI1140
  660 SWAP=A(K,JROW)                                          MATI1150
  670 A(K,JROW)=A(K,JCOLUM)                                   MATI1160
  700 A(K,JCOLUM)=SWAP                                        MATI1170
  705 CONTINUE                                                MATI1180
  710 CONTINUE                                                MATI1190
  740 RETURN                                                  MATI1200
      END                                                     MATI1210
```

```
      SUBROUTINE FGH(N,F,G,H)
C  **     **     FIRST DERIVATIVE    **     **     **
C------EVALUATES COEFFICIENTS FOR THREE POINT DIFFERENCE APPROXIMATION
C      OF DAVIS (AIAA JR. VOL. 8, NO. 5, MAY 1970).
      COMMON /YL/ETA(60),YOND(60)
      DN=ETA(N+1)-ETA(N)
      DNM1=ETA(N)-ETA(N-1)
      DEL=DN+DNM1
      D1=DN*DEL
      D2=DN*DNM1
      D3=DNM1*DEL
      F=DNM1/D1
      G=(DN-DNM1)/D2
      H=-DN/D3
      RETURN
      END
```

```
      SUBROUTINE FGH2(N,F,G,H)
C  **    **    SECOND DERIVATIVE    **    **    **
C------EVALUATES COFFFICIENTS FOR THREE POINT DIFFERENCE APPROXIMATION
C       OF DAVIS (AIAA JR. VOL. 8, NO. 5, MAY 1970).
      COMMON /YL/ETA(60),YOND(60)
      DN=ETA(N+1)-ETA(N)
      DNM1=ETA(N)-ETA(N-1)
      F=2./(DN*(DN+DNM1))
      G=-2./(DN*DNM1)
      H=2./(DNM1*(DN+DNM1))
      RETURN
      END
```

```
      SUBROUTINE TRID (M)
C**** TRID --TRIDIAGONAL EQUATION SOLVER  OBTAINED FROM CONTE P-184 ***
C      SUBROUTINE SOLVES AX = B FOR THE VECTOR X (WHERE A IS TRIDIAGONAL
C      M = ORDER OF SYSTEM
C      SUP = SUPER DIAGONAL OF A
C      SUB = SUB DIAGONAL OF A
C      DIAG = MAIN DIAGONAL OF A
C      B = CONSTANT VECTOR
C      SUP AND DIAG ARE DESTROYED
C      SOLUTION VECTOR IS RETURNED IN B
C
      COMMON/VECTOR/ SUB(60),DIAG(60),SUP(60),B(60)
C
      N = M
      NN = N -1
      SUP(1) = SUP(1)/DIAG(1)
      B(1) = B(1)/DIAG(1)
      DO 10 I=2,N
      II = I -1
C------DECOMPOSE A TO FORM A = LU WHERE L IS LOWER TRIANGULAR,
C      AND U IS UPPER TRIANGULAR ---------
      DIAG(I) = DIAG(I) - SUP(II)*SUB(II)
      IF(I .EQ. N) GO TO 10
      SUP(I) = SUP(I) / DIAG(I)
C------COMPUTE Z WHERE LZ = B
   10 B(I) = (B(I) - SUB(II) *B(II))/ DIAG(I)
C------COMPUTE X BY BACK SUBSTITUTION WHERE UX = Z
      DO 20 K =1,NN
      I = N - K
   20 B(I) = B(I) -SUP(I) *B(I+1)
      RETURN
      END
```

```
      FUNCTION QUAD (X,FX,I)
C
C     **  TRAPEZOIDAL QUADRATURE FUNCTION  **
C
      DIMENSION X(60),FX(60)
      DX=X(I)-X(I-1)
      QUAD = (DX/2.0) * (FX(I) + FX(I-1) )
      RETURN
      END
```

```
      SUBROUTINE OUTPUT(N)
C
C
C     **  ROUTINE TO PRINT SHOCK LAYER SOLUTION  **
C
C
      COMMON/ID/SP(20),EL(5)
      COMMON /CONV/ FPRCT,TPRCT,DDAMP,TDAMP,PDTIL
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /FRSTRM/ U INF, 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,NNS,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,ITYPE
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON /SFLUX/QRI(3)
      COMMON/VECTOR/ CA(60),CB(60),CC(60),B(60)
      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 /DY/ DYDT(20,60)
      DIMENSION BOUT(60),DQR(30)
      REAL  MU,MUDZ
      DATA HEAD1/'WALL'/ ,HEAD2/'    '/,HEAD3/'SHOC'/
C
C
C     **  COMPUTE RADIATION FLUX IF UNCOUPLED PROBLEM  **
C
      IF(ITYPE.NE.0)GOTO20
      IF(IRAD .EQ. 2  .AND.  N .NE. 2) CALL TRANS(1)
      IF (IRAD.NE.1) CALL TRANS2
   20 IF(IRAD.EQ.2.AND.ITYPE.EQ.1) CALL EFLUX
      WRITE(6,203)
```

```
  203 FORMAT(1H1)
C
C      **  COMPUTE Y COORDINATE  **
C
       YOND(1) = 0.0
       SUM = 0.0
       DO 40 K=2,NETA
       DETA= ETA(K)-ETA(K-1)
       SUM= SUM +DETA*(1./RHO(K)+1./RHO(K-1))/2.
       YOND(K) = DTIL*SUM
  40   CONTINUE
       DELTA = YOND(NETA)
       DO 50 K=1,NETA
       YOND(K)= YOND(K)/DELTA
  50   CONTINUE
C
C      **  COMPUTE CONVECTIVE HEATING RATE  **
C
C WATTS/CM**3
       QC = -AK(1)*RINF*UINF*UINF2*   (T(2)-T(1))/
     1  (.88*778.28        *YOND(2)*DELTA*RZB)
C BTU/FT**2-SEC
       QCP=QC*.88
C
C      **  COMPUTE RADIATIVE FLUX TO SURFACE  **
C
       QR = 0.0
       IF(IRAD .EQ. 1) GO TO 445
       DO 1100 K=2,NETA
       QR = QR + QUAD(YOND,E,K)
 1100  CONTINUE
C WATTS/CM**2
       QR =-QR *RINF*UINF2*UINF *DELTA/(685.*RZB)
       IF(ITYPE.EQ.0)QR=-QRI(1)
 445   CONTINUE
C BTU/FT**2-SEC
```

```
      QRP=QR*0.98
      QTOTAL=QC+QR
      QTOTP=QTOTAL*.98
      QCZ=QC
      QRZ=QR
      QTZ=QTOTAL
      QCRAT = 1.0
      IF(QC.LT.0.0) QCRAT= QC/QCZ
      QRRAT = 1.0
      IF(QR.LT. 0.0) QRRAT = QR/QRZ
      QTRAT=1.0
C
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
  450 CONTINUE
C
C     **  CORRELATION FORMULAS FOR OUTPUT   **
C
      QKR=16000.0*SQRT(RINF)*(UINF/10000.0)**3.25
      QKR=-QKR/SQRT(R)
      HIS=HTOTAL/(32.174*778.0)
      SRENU=0.763*(PRW      )**0.4 * (RM(NETA)/RM(1) )**0.4
      PS=PD*2116.0
      RS=RHO(NETA)
      DUEDX=(1.0/R)*SQRT(2.0*PS/RS)
      SDUEDX=SQRT(DUEDX      )
      SRMPR=SQRT(RM(1    ))*32.174/PRW
      QFR=-SRENU*SRMPR*SDUEDX*HIS
      QRT=-495000.0*RINF**1.98*(UINF/10000.0)**14*R
```

```
      QT=QRT+QKP
      RLAMBA=QRP/(RINF*UINF**3/(2.*778.28))
C
      GO TO  (1,2,3,4) , N
C
 1    WRITE(6,201) IEM
 201  FORMAT(23H SOLUTION CONVERGED IN  ,I3,11H ITERATIONS //)
      GO TO 4
C
 2    WRITE (6,202) IEM
 202  FORMAT(1H0,37H INTERMEDIATE PRINT AT ITERATION NO. ,I4,//)
      GO TO 4
C
    3 CONTINUE
C
 4    CONTINUE
C
C     **  PRINT SHOCK QUANTITIES AND HEATING RATE  **
C
      XID=0.0
      WRITE(6,204) XID,DELTA,DTIL
  204 FORMAT(1H0,7H XI   = ,F9.4, 9X,9H DELTA = ,1PE14.6,10X,7HDTIL = ,
     1    E15.6)
C
      EPSOT = 0.0
      WRITE (6,210) EPSOT,QC,QCP
 210  FORMAT ( 1H0,7H EPS = ,F9.4,9X,5H QC = E15.6,2X,13H(WATTS/CM**2),
     1          2X,1H=,E15.6,2X,17H(BTU/FT**2 - SEC)        )
      WRITE(6,212) RZB,QR,QRP
 212  FORMAT ( 1H0,6H RB  =,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,QKR,QFR
 213  FORMAT(1H0,6H RVW= ,F9.4,10X,6H QKR = E14.6,12X,6H QFR = E15.6)
      WRITE (6,214) QRT,QT,RLAMBA
  214 FORMAT (1H ,25X,6H QRT =E14.6,12X,6H QT  = E15.6,8X,
     1       9HLAMBDA = ,E15.6)
```

```
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)      )
      WRITE(6,216) QCRAT,QRRAT,QTRAT
  216 FORMAT(21HCHEATING DISTRIBUTION   ,
     1              5X,9H QC/QCZ = E14.6,2X,8HQR/QRZ = E14.6,2X,
     1                 8HQT/QTZ = E14.6  ////)
C
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        4HT/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
      IF(IEM.LT.IAB) NS=7
      HSTAT = 0.0
      DO 99 J=1,NS
   99 HSTAT = HSTAT + HS(J,I)*C(J,I)
      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*2.
      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 ,A4,  F6.3,1P10E12.3)
      IF(I.LT.NETA-1) FP = Z(I)*DTIL
```

```
  100 CONTINUE                                                          OUTP1810
C                                                                       OUTP1820
C     **  WRITE OUT SHOCK LAYER GAS PROPERTIES   **                     OUTP1830
C                                                                       OUTP1840
      WRITE(6,44)                                                       OUTP1850
 44   FORMAT(1H1,48X,28H-SHOCK LAYER GAS PROPERTIES-    )               OUTP1860
C                                                                       OUTP1870
      WRITE(6,206)                                                      OUTP1880
 206  FORMAT(1H0,3X,3HETA,8X,4H Y/D,12X,2HP ,12X,2H T,11X,3HRHO,11X,2HMUOUTP1890
     1         , 12X, 3HRMU,11X,2H K)                                   OUTP1900
C                                                                       OUTP1910
      WRITE(6,207)                                                      OUTP1920
 207  FORMAT (1H ,27X,6H(ATM.),6X,13H (DEG.KEL.)  ,12H(SLUGS/FT3) ,2X,  OUTP1930
     1         28H(LBM/FT-SEC) (LBF2-SEC3/FT6) ,16H (BTU/FT-SEC-R) ,//) OUTP1940
C                                                                       OUTP1950
      DO 101 I=1,NETA                                                   OUTP1960
C                                                                       OUTP1970
      TS = T(I)*TD                                                      OUTP1980
      WRITE(6,8)ETA(I),YOND(I),PI(I),TS  ,RHO(I),MU(I),RM (I),AK(I)     OUTP1990
C                                                                       OUTP2000
    8 FORMAT(1H F7.4,1P8E14.4)                                          OUTP2010
    9 FORMAT(1H F7.4,1P7E14.4)                                          OUTP2020
C                                                                       OUTP2030
  101 CONTINUE                                                          OUTP2040
C                                                                       OUTP2050
C     **  WRITE SPECIES MASS FRACTIONS  **                              OUTP2060
C                                                                       OUTP2070
      WRITE(6,230)                                                      OUTP2080
 230  FORMAT (1H1,48X,26H-SPECIES MASS FRACTIONS-    )                  OUTP2090
      WRITE(6,231)                                                      OUTP2100
 231  FORMAT (1H ,14X,3H O2,11X,2HN2,11X,3H O ,11X,3H N ,11X,3H O+,     OUTP2110
     1        11X,3H N+,11X,3H E-,//)                                   OUTP2120
      DO 102 I=1,NETA                                                   OUTP2130
      WRITE(6,8) ETA(I),C(1,I),C(2,I),C(3,I),C(4,I),C(5,I),             OUTP2140
     1        C(6,I),C(7,I)                                             OUTP2150
  102 CONTINUE                                                          OUTP2160
```

```
      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 NONDIMENSIONALIZE
      DO1001I=1,NETA
      RHO(I) = RHO(I)/RDZ
      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
      WRITE(7,217) (T  (I),I=1,NETA)
      WRITE (7,217) (RHO(I),I=1,NETA)
      WRITE (7,217) (RM (I),I=1,NETA)
      WRITE(7,217) (ETA(I),I=1,NETA)
  217 FORMAT(6E12.5)
 1000 CONTINUE
C
      RETURN
C
      END
```

```
      SUBROUTINE ERROR  ( N )
C
      IF(N .EQ. 1 ) WRITE(6,1 )
C
      IF(N .EQ. 2 ) WRITE(6,2 )
C
      IF(N .EQ. 3) WRITE(6,3)
C
C
      RETURN
C
 1    FORMAT(36H1 MOMENTUM EQUATION DID NOT  CONVERGE      )
 2    FORMAT(34H1 ENERGY EQUATION DID NOT CONVERGE      )
 3    FORMAT(54H MOMENTUM AND ENERGY FAILED TO CONVERGE SIMULTANEOUSLY )
      END
```

```
      SUBROUTINE ELPROF
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NT
      COMMON /VEL/ F(60),FC(60),Z(60),VV(60)
      COMMON /YL/ ET(60),YOND(60)
      COMMON/PROP1/PI(60),RO(60),TT(60),AMW(60),C (20,60),CC(5,60)
      DOUBLE PRECISION NAME(9)
      DATA NAME/' CARBON ','HYDROGEN','NITROGEN',' OXYGEN ','ELECTRON',
     1          '  T(OK)  ','VELOCITY','   Y/D    ',' DENSITY'/
      PRINT 103
      PRINT 100,NAME
      DO5N=1,NT
5     PRINT 101,ET(N),(CC(I,N),I=1,5),TT(N),VV(N),YOND(N),RO(N)
      RETURN
100   FORMAT(     5X,'ETA',3X,9(2X,A8,2X))
101   FORMAT(F10.4,1X,9E12.4)
103   FORMAT( 15X,14('*'),'ELEMENTAL MASS FRACTIONS',15('*'))
      END
```

```
      SUBROUTINE MULTI                                                   MULT  10
      COMMON /DEL/ DELTA,DTIL,DTILS                                      MULT  20
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA     MULT  30
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL                           MULT  40
      COMMON /YL/ ET( 60),YOND( 60)                                      MULT  50
      COMMON /VEL/ F( 60),FC( 60),ZZ( 60),VV( 60)                        MULT  60
      COMMON/PROP1/PI( 60),RO( 60),TT( 60),AMW( 60),C (20, 60),CC(5, 60)MULT  70
      COMMON/NUMBER/NSP,NNS,NE,NC                                        MULT  80
C                                                                        MULT  90
C     PUNCHES DATA PKG. FOR MULTICOMPONENT DIFFUSION  ANALYSIS           MULT 100
C                                                                        MULT 110
      M=7                                                                MULT 120
      TOL=.01                                                            MULT 130
      RINF=RINF*32.164                                                   MULT 140
      DO10N=1,NETA                                                       MULT 150
      TT(N)=TT(N)*TD                                                     MULT 160
   10 VV(N)=VV(N)*UINF                                                   MULT 170
C                                                                        MULT 180
      WRITE(M,100)NETA,NSP,NE,NSP                                        MULT 190
      WRITE(M,101)TOL,UINF,DTIL,RAD,RINF,RZB,DELTA                       MULT 200
C                                                                        MULT 210
      WRITE(M,102)(  ET(N),N=1,NETA)                                     MULT 220
      WRITE(M,102)(YOND(N),N=1,NETA)                                     MULT 230
      WRITE(M,102)(  TT(N),N=1,NETA)                                     MULT 240
      WRITE(M,102)(  PI(N),N=1,NETA)                                     MULT 250
      WRITE(M,102)(  VV(N),N=1,NETA)                                     MULT 260
      WRITE(M,102)(  RO(N),N=1,NETA)                                     MULT 270
C                                                                        MULT 280
      RETURN                                                             MULT 290
  100 FORMAT(5X,2I5,5X,2I5)                                              MULT 300
  101 FORMAT(8E10.4)                                                     MULT 310
  102 FORMAT(6E12.4)                                                     MULT 320
      END                                                                MULT 330
```

```
      BLOCK DATA
      COMMON/FINV/ NHVL,NIHVC,FHVC(12),DJ(9),HVJ(9),ZKZ
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON/GUESS/TG1(60),TG2(60)
      COMMON/PROP1/PI(60),RHO(60), T(60),AMW(50),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/NUMBER/NSP,NNS,NE,NC
      COMMON/ELSP/LSP(5)
      COMMON/ID/SP(20),EL(5)
      COMMON/WT/SMW(20),AWT(5)
      COMMON /BLOCK1/V1(20),V2(20),V3(20)
      COMMON/BLOCK3/K1(20),K2(20)
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/EQ2/AA(20,5),ICODE(20)
      COMMON/EQ3/IA(20,5)
      REAL K1,K2
      DATA NETA/0/
      DATA RHO /25.1,14.3,8.85,6.50,4.37,3.01,2.49,2.17,1.90,1.67,1.46,
     1          1.29,1.16,1.08,1.03,1.00,44*1.0/
      DATA RM /10.0,7.71,5.89,5.10,4.18,3.54,3.31,3.10,2.83,2.48,2.09,
     1         1.72,1.42,1.22,1.09,1.02,44*1.0/
      DATA TG1 / .1033,.2294,.3531,.4719,.5777,.6531,.6867,.7034,.7145,
     1 .7236,.7321,.7401,.7479,.7554,.7628,.7699,.7769,.7836,.7902,
     2 .7967,.8030,.8092,.8153,.8213,.8272,.8331,.8389,.8447,.8504,
     3 .8562,.8619,.8676,.8734,.8791,.8850,.8908,.8968,.9028,.9089,
     4 .9151,.9215,.9280,.9347,.9417,.9488,.9563,.9641,.9723,.9809,
     5 .9901,10*1.0/
      DATA TG2 / .3325,.3325,.3325,.3325,.3325,.3325,.3325,.3326,.3328,
     1 .3331,.3336,.3344,.3357,.3378,.3408,.3452,.3515,.3601,.3718,
     2 .3873,.4076,.4335,.4665,.5075,.5560,.6054,.6487,.6857,.7161,
     3 .7404,.7595,.7749,.7878,.7993,.8100,.8203,.8302,.8399,.8496,
     4 .8594,.8693,.8797,.8904,.9019,.9142,.9278,.9476,.9609,.9757,
     5 .9877,10*1.0/
C
```

```
      DATA NSP,NNS,NE,NC/20,0,5,20/                                     DATA 370
      DATA SP/ 'O2  ',   'N2  ',   'O   ',   'N   ',   'O+  ',          DATA 380
     1         'N+  ',   'E-  ',   'C   ',   'H   ',   'H2  ',          DATA 390
     2         'CO  ',   'C3-G',   'CN  ',   'C2H ',   'C2H2',          DATA 400
     3         'C3H ',   'C4H ',   'HCN ',   'C2  ',   'C+  '/          DATA 410
C                                                                       DATA 420
      DATA SMW/32.000,   28.016,   16.000,   14.008,   16.000,          DATA 430
     1         14.008, 5.486E-4,   12.011,    1.008,    2.016,          DATA 440
     2         28.011,   36.033,   26.019,   25.030,   26.038,          DATA 450
     3         37.041,   49.052,   27.027,   24.022,   12.011/          DATA 460
C                                                                       DATA 470
      DATA V1/0.1693E 01,0.9704E 00,0.1519E 01,0.2534E 00,0.0         , DATA 480
     1        0.0       ,0.0       ,0.1997E 01,0.2941E 00,-.7944E-01,  DATA 490
     2        0.2404E 01,0.2019E 01,0.2404E 01,0.2404E 01,0.1396E 01,  DATA 500
     3        0.2019E 01,0.2019E 01,0.1378E 01,0.1931E 01,0.0        /  DATA 510
C                                                                       DATA 520
      DATA V2/0.1496E-02,0.1613E-02,0.1875E-02,0.2206E-02,0.5000E-03,  DATA 530
     1        0.5000E-03,0.5000E-03,0.1772E-02,0.8893E-03,0.7907E-03,  DATA 540
     2        0.1363E-02,0.1179E-02,0.1363E-02,0.1363E-02,0.8423E-03,  DATA 550
     3        0.1179E-02,0.1179E-02,0.9651E-03,0.1393E-02,0.5000E-03/  DATA 560
C                                                                       DATA 570
      DATA V3/-.2276E-07,-.1916E-07,-.2228E-07,-.3737E-07,-.1000E-07,  DATA 580
     1        -.1000E-07,-.1000E-07,-.3378E-07,-.8111E-08,-.8864E-08,  DATA 590
     2        -.2184E-07,-.1655E-07,-.2184E-07,-.2184E-07,-.6939E-08,  DATA 600
     3        -.1655E-07,-.1655E-07,-.9481E-08,-.2575E-07,-.1000E-07/  DATA 610
C                                                                       DATA 620
      DATA  AI/0.3316E 01,0.3221E 01,0.2670E 01,0.2474E 01,0.2491E 01,  DATA 630
     1         0.2727E 01,0.2500E 01,0.2612E 01,0.2500E 01,0.3358E 01,  DATA 640
     2         0.3254E 01,0.4002E 01,0.3411E 01,0.3485E 01,0.3891E 01,  DATA 650
     3         0.3965E 01,0.5874E 01,0.3654E 01,0.4443E 01,0.2609E 01/  DATA 660
C                                                                       DATA 670
      DATA  BI/0.1151E-02,0.9878E-03,-.1970E-03,0.9097E-04,0.2762E-04,  DATA 680
     1         -.2820E-03,0.3440E-06,-.2030E-03,-.8243E-06,0.2794E-03,  DATA 690
     2         0.9698E-03,0.3541E-02,0.4897E-03,0.3563E-02,0.5717E-02,  DATA 700
     3         0.6200E-02,0.7403E-02,0.3444E-02,-.2385E-03,-.1393E-03/  DATA 710
C                                                                       DATA 720
```

```
      DATA  CI/-.3726E-06,-.2907E-06,0.7193E-07,-.7814E-07,-.1881E-07,   DATA 730
     1         0.1105E-06,-.1954E-09,0.1095E-06,0.6421E-09,0.9372E-07,   DATA 740
     2         -.2647E-06,-.1318E-05,0.1005E-06,-.1237E-05,-.1957E-05,   DATA 750
     3         -.2265E-05,-.2729E-05,-.1258E-05,0.3036E-06,0.5959E-07/   DATA 760
C                                                                        DATA 770
      DATA  DI/0.6186E-10,0.3938E-10,-.8901E-11,0.2218E-10,0.3807E-11,   DATA 780
     1         -.1551E-10,0.3937E-13,-.1695E-10,-.1720E-12,-.2948E-10,   DATA 790
     2         0.3037E-10,0.2064E-09,-.3473E-10,0.1866E-09,0.2931E-09,   DATA 800
     3         0.3717E-09,0.4437E-09,0.2169E-09,-.6244E-10,-.1037E-10/   DATA 810
C                                                                        DATA 820
      DATA  EI/-.3666E-14,-.2000E-14,0.4002E-15,-.1489E-14,-.1028E-15,   DATA 830
     1         0.7847E-15,-.2573E-17,0.8590E-15,0.1457E-16,0.2141E-14,   DATA 840
     2         -.1177E-14,-.1144E-13,0.2361E-14,-.1013E-13,-.1585E-13,   DATA 850
     3         -.2262E-13,-.2537E-13,-.1430E-13,0.3915E-14,0.6345E-15/   DATA 860
C                                                                        DATA 870
      DATA  FI/-.1044E 04,-.1043E 04,0.2915E 05,0.5609E 05,0.1879E 06,   DATA 880
     1         0.2254E 06,-.7450E 03,0.8542E 05,0.2547E 05,-.1018E 04,   DATA 890
     2         -.1434E 05,0.9423E 05,0.4745E 05,0.5809E 05,0.2590E 05,   DATA 900
     3         0.6283E 05,0.7605E 05,0.1442E 05,0.9787E 05,0.2168E 06/   DATA 910
C                                                                        DATA 920
      DATA  GI/0.5393E 01,0.4326E 01,0.4504E 01,0.4300E 01,0.4424E 01,   DATA 930
     1         0.3645E 01,-.1173E 02,0.4144E 01,-.4612E 00,-.3548E 01,   DATA 940
     2         0.4875E 01,0.2020E 01,0.4746E 01,0.4784E 01,0.6520E 00,   DATA 950
     3         0.3467E 01,-.4010E 01,0.2373E 01,-.1090E 01,0.3709E 01/   DATA 960
C                                                                        DATA 970
      DATA AII/0.3721E 01,0.3727E 01,0.2546E 01,0.2746E 01,0.2944E 01,   DATA 980
     1         0.2499E 01,0.2508E 01,0.2141E 01,0.3934E 01,0.3363E 01,   DATA 990
     2         0.3366E 01,0.2213E 02,0.3473E 01,0.5307E 01,0.6789E 01,   DATA1000
     3         0.3965E 01,0.5874E 01,0.3654E 01,0.4026E 01,0.2528E 01/   DATA1010
C                                                                        DATA1020
      DATA BII/0.4254E-03,0.4684E-03,-.5952E-04,-.3909E-03,-.4108E-03,   DATA1030
     1         -.3725E-05,-.6332E-05,0.3219E-03,-.1776E-02,0.4656E-03,   DATA1040
     2         0.8027E-03,-.1759E-01,0.7337E-03,0.8966E-03,0.1503E-02,   DATA1050
     3         0.6200E-02,0.7403E-02,0.3444E-02,0.4857E-03,0.4869E-05/   DATA1060
C                                                                        DATA1070
      DATA CII/-.2835E-07,-.1140E-06,0.2701E-07,0.1338E-06,0.9156E-07,   DATA1080
```

```
     1          0.1147E-07,0.1364E-08,-.5498E-07,0.6013E-06,-.5127E-07,   DATA1090
     2          -.1968E-06,0.5565E-05,-.9088E-07,-.1378E-06,-.2295E-06,   DATA1100
     3          -.2265E-05,-.2729E-05,-.1258E-05,-.7026E-07,-.7026E-08/   DATA1110
C                                                                         DATA1120
      DATA DII/0.6050E-12,0.1154E-10,-.2798E-11,-.1191E-10,-.5848E-11,   DATA1130
     1          -.1102E-11,-.1094E-12,0.3604E-11,-.7819E-10,0.2802E-11,   DATA1140
     2          0.1940E-10,-.6758E-09,0.4847E-11,0.9251E-11,0.1534E-10,   DATA1150
     3          0.3717E-09,0.4437E-09,0.2169E-09,0.4666E-11,0.1134E-11/   DATA1160
C                                                                         DATA1170
      DATA EII/-.5186E-17,-.3293E-15,0.9380E-16,0.3369E-15,0.1190E-15,   DATA1180
     1          0.3078E-16,0.2934E-17,-.5564E-16,0.3482E-14,-.4905E-16,   DATA1190
     2          -.5549E-15,0.2825E-13,-.1018E-15,-.2278E-15,-.3763E-15,   DATA1200
     3          -.2262E-13,-.2637E-13,-.1430E-13,-.1142E-15,-.3476E-16/   DATA1210
C                                                                         DATA1220
      DATA FII/-.1044E 04,-.1043E 04,0.2915E 05,0.5609E 05,0.1879E 06,   DATA1230
     1          0.2254E 06,-.7450E 03,0.8542E 05,0.2547E 05,-.1018E 04,   DATA1240
     2          -.1434E 05,0.9423E 05,0.5420E 05,0.5809E 05,0.2590E 05,   DATA1250
     3          0.6283E 05,0.7605E 05,0.1442E 05,0.9787E 05,0.2168E 06/   DATA1260
C                                                                         DATA1270
      DATA GII/0.3254E 01,0.1294E 01,0.5049E 01,0.2872E 01,0.1750E 01,   DATA1280
     1          0.4950E 01,-.1208E 02,0.6874E 01,-.8598E 01,-.3716E 01,   DATA1290
     2          0.4263E 01,-.1021E 03,0.4152E 01,-.5288E 01,-.1539E 02,   DATA1300
     3          0.3467E 01,-.4010E 01,0.2373E 01,0.1090E 01,0.4139E 01/   DATA1310
C                                                                         DATA1320
      DATA K1/0.1019E 01,0.6541E 00,0.1250E 01,0.1281E 01,2.6000E 01,    DA
     1         2.6000E 01,2.6000E 01,0.2506E 01,0.2496E 01,0.3211E 01,    DATA
     2         0.8589E 00,0.6304E 00,0.8589E 00,0.1126E 01,0.1126E 01,    DATA1350
     3         0.6304E 00,0.6304E 00,0.4855E 00,0.8589E 00,0.1000E-04/    DATA1360
C                                                                         DATA1370
      DATA K2/0.4901E-03,0.6457E-03,0.7092E-03,0.8593E-03,0.0000E-03,    DAT
     1         0.0000E-03,0.0000E-03,0.7479E-03,0.5129E-02,0.5344E-02,    DATA
     2         0.6233E-03,0.5804E-03,0.6233E-03,0.7439E-03,0.7439E-03,    DATA1400
     3         0.5804E-03,0.5804E-03,0.8714E-03,0.6233E-03,0.7350E-03/    DATA1410
C                                                                         DATA1420
      DATA ICODE/20*0/                                                    DATA1430
C                                                                         DATA1440
```

```
      DATA FL/    'C',     'H',     'N',     'O',     'E'   /           DATA1450
      DATA AWT/ 12.011,  1.008,  14.008, 16.000, 5.486E-4   /           DATA1460
C                                                                       DATA1470
      DATA IA/ 0,0,0,0,0,0,0,1,0,0,1,3,1,2,2,3,4,1,2,1,                 DATA1480
     H         0,0,0,0,0,0,0,0,1,2,0,0,0,1,2,1,1,1,0,0,                 DATA1490
     N         0,2,0,1,0,1,0,0,0,0,0,0,1,0,0,0,0,1,0,0,                 DATA1500
     O         2,0,1,0,1,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,                 DATA1510
     E         2,2,1,1,0,0,1,1,0,0,2,3,2,2,2,3,4,2,2,0/                 DATA1520
C                                                                       DATA1530
      DATA LSP/20,9,6,5,7/                                              DATA1540
      DATA NHVL /9/, NIHVC /12/                                         DATA1550
      DATA FHVC /5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 10.8, 11.1,             DATA1560
     1   12.0, 13.4, 14.3, 20.0/                                        DATA1570
      DATA DJ /0.6, 2.2, 1.5, 1.65, 1.4, 1.0, 1.2, 1.4, 1.0/            DATA1580
      DATA HVJ /1.3, 2.7, 5.75, 7.57, 9.1, 10.4, 11.4, 12.7, 13.9/      DATA1590
      DATA ZKZ /7.26E-16/                                               DATA1600
      END                                                               DATA1610
```

```
0.05 BLOWING CASE    0.1 ATMOSPHERE
      59    3               15            2
     50000.       8.85E-6          9.          3450.                    0.05

0.26543E 00 0.26995E 00 0.27470E 00 0.27972E 00 0.28505E 00 0.28855E 00
0.29220E 00 0.29600E 00 0.29998E 00 0.30413E 00 0.30846E 00 0.31771E 00
0.33187E 00 0.34731E 00 0.36387E 00 0.38144E 00 0.39192E 00 0.40829E 00
0.42539E 00 0.44927E 00 0.47403E 00 0.49951E 00 0.52554E 00 0.55146E 00
0.57621E 00 0.59891E 00 0.61933E 00 0.65350E 00 0.66844E 00 0.68234E 00
0.69555E 00 0.70835E 00 0.73310E 00 0.75734E 00 0.78036E 00 0.81150E 00
0.82929E 00 0.85139E 00 0.87347E 00 0.88234E 00 0.89646E 00 0.90210E 00
0.91165E 00 0.91591E 00 0.92002E 00 0.92797E 00 0.93172E 00 0.93903E 00
0.94263E 00 0.94959E 00 0.95309E 00 0.96002E 00 0.96350E 00 0.97049E 00
0.97411E 00 0.98153E 00 0.98559E 00 0.99414E 00 0.10000E 01
0.52986E 01 0.50182E 01 0.47433E 01 0.44748E 01 0.42130E 01 0.40541E 01
0.38998E 01 0.37507E 01 0.36077E 01 0.34722E 01 0.33445E 01 0.31150E 01
0.28532E 01 0.26514E 01 0.24894E 01 0.23484E 01 0.22723E 01 0.21612E 01
0.20533E 01 0.19154E 01 0.17873E 01 0.16772E 01 0.15902E 01 0.15247E 01
0.14757E 01 0.14397E 01 0.14146E 01 0.13923E 01 0.13903E 01 0.13931E 01
0.13994E 01 0.14080E 01 0.14293E 01 0.14502E 01 0.14684E 01 0.14860E 01
0.14900E 01 0.14837E 01 0.14565E 01 0.14381E 01 0.13970E 01 0.13781E 01
0.13424E 01 0.13257E 01 0.13098E 01 0.12799E 01 0.12654E 01 0.12386E 01
0.12253E 01 0.12003E 01 0.11876E 01 0.11636E 01 0.11514E 01 0.11281E 01
0.11161E 01 0.10919E 01 0.10792E 01 0.10525E 01 0.10351E 01
0.34337E 01 0.32770E 01 0.31214E 01 0.31319E 01 0.29706E 01 0.28707E 01
0.28975E 01 0.27958E 01 0.26961E 01 0.27112E 01 0.26137E 01 0.25520E 01
0.24419E 01 0.23690E 01 0.23213E 01 0.22873E 01 0.22183E 01 0.22474E 01
0.22229E 01 0.21803E 01 0.21402E 01 0.20982E 01 0.20680E 01 0.20496E 01
0.20379E 01 0.20308E 01 0.20279E 01 0.20414E 01 0.20552E 01 0.20735E 01
0.20951E 01 0.21183E 01 0.21672E 01 0.22092E 01 0.22393E 01 0.22498E 01
0.22333E 01 0.21791E 01 0.20745E 01 0.20493E 01 0.18995E 01 0.18744E 01
0.17535E 01 0.17320E 01 0.17115E 01 0.15937E 01 0.15758E 01 0.15427E 01
0.14571E 01 0.14274E 01 0.14122E 01 0.13065E 01 0.12927E 01 0.12666E 01
0.11953E 01 0.11693E 01 0.11557E 01 0.10526E 01 0.10351E 01
0.0         0.50000E-02 0.10000E-01 0.15000E-01 0.20000E-01 0.23125E-01
0.26250E-01 0.29375E-01 0.32500E-01 0.35625E-01 0.38750E-01 0.45000E-01
```

0.53750E-01	0.62500E-01	0.71250E-01	0.80000E-01	0.85000E-01	0.92500E-01
0.10000E 00	0.11000E 00	0.12000E 00	0.13000E 00	0.14000E 00	0.15000E 00
0.16000E 00	0.17000E 00	0.18000E 00	0.20000E 00	0.21000E 00	0.22000E 00
0.23000E 00	0.24000E 00	0.26000E 00	0.28000E 00	0.30000E 00	0.33000E 00
0.35000E 00	0.38000E 00	0.42000E 00	0.44000E 00	0.48000E 00	0.50000E 00
0.54000E 00	0.56000E 00	0.58000E 00	0.62000E 00	0.64000E 00	0.68000E 00
0.70000E 00	0.74000E 00	0.76000E 00	0.80000E 00	0.82000E 00	0.86000E 00
0.88000E 00	0.92000E 00	0.94000E 00	0.98000E 00	0.10000E 01	

1.CE-10	.02389	1.0E-10	2.0E-05	1.0E-10
1.0E-10	1.0E-10	.00157	.01708	.03277
.25780	.01767	.00310	.15000	.08216
.20370	.15890	.04710	.00413	1.0E-10

```
                                      1  C        2  H        3  N        4  O        5  E
NO. SPECIES   =    20
                                      1  O2       2  N2       3  O        4  N        5  O+
                                      6  N+       7  E-       8  C        9  H       10  H2
                                     11  CO      12  C3-G    13  CN      14  C2H     15  C2H2
                                     16  C3H     17  C4H     18  HCN     19  C2      20  C+
NO. SOLIDS    =     0

SPECIES
NAME             SMW  WALL MASS FRACTION

O2            32.000  0.1000E-09
N2            28.016  0.2389E-01
O             16.000  0.1000E-09
N             14.008  0.2000E-04
O+            16.000  0.1000E-09
N+            14.008  0.1000E-09
E-             0.001  0.1000E-09
C             12.011  0.1570E-02
H              1.008  0.1708E-01
H2             2.016  0.3277E-01
CO            28.011  0.2578E 00
C3-G          36.033  0.1767E-01
CN            26.019  0.3100E-02
C2H           25.030  0.1500E 00
C2H2          26.038  0.8216E-01
C3H           37.041  0.2037E 00
C4H           49.052  0.1589E 00
HCN           27.027  0.4710E-01
C2            24.022  0.4130E-02
C+            12.011  0.1000E-09

DENSITY RATIO      REYNOLDS NO.
  0.536357E-01    0.311032E 06

DELTA              DTIL
  0.418359E-01    0.106019E 00
```

```
0.05 BLOWING CASE   0.1 ATMOSPHERE


INPUT DATA


KEEP    =    0
NETA    =   59
MAXM    =   15
MAXE    =   15
MAXD    =   15
FPRCT   =   4.999999E-03
TPRCT   =   4.999999E-03
LT      =    2
IDEBUG  =    0
IPHI    =    0

UINF    =   5.000000E 04
RINF    =   8.849997E-08
R       =   9.000000E 00
TW      =   3.450000E 03
HTOTAL  =   1.250000E 09
RVW     =   5.000000E-02
DXI     =   0.0
PDTIL   =   9.999999E-04

* COUPLED RADIATION CALCULATION *
* CONTINUUM AND LINE CALCULATION *

INITIAL T PROFILE
   0.26543   0.26995   0.27470   0.27972   0.28505   0.28855   0.29220   0.29600   0.29998   0.30413   0.30846   0.31771
   0.33187   0.34731   0.36387   0.38144   0.39192   0.40829   0.42539   0.44927   0.47403   0.49951   0.52554   0.55146
   0.57621   0.59891   0.61933   0.65350   0.66844   0.68234   0.69555   0.70835   0.73310   0.75734   0.78036   0.81150
   0.82929   0.85139   0.87347   0.88234   0.89646   0.90210   0.91165   0.91591   0.92002   0.92797   0.93172   0.93903
   0.94263   0.94959   0.95309   0.96002   0.96350   0.97049   0.97411   0.98153   0.98559   0.99414   1.00000

INITIAL RHO PROFILE
   5.29860   5.01820   4.74330   4.47480   4.21300   4.05410   3.89980   3.75070   3.60770   3.47220   3.34450   3.11500
   2.85320   2.65140   2.48940   2.34840   2.27230   2.16120   2.05330   1.91540   1.78730   1.67720   1.59020   1.52470
   1.47570   1.43970   1.41460   1.39230   1.39030   1.39310   1.39940   1.40800   1.42930   1.45020   1.46840   1.48600
   1.49000   1.48370   1.45650   1.43810   1.39700   1.37810   1.34240   1.32570   1.30980   1.27990   1.26540   1.23660
   1.22530   1.20030   1.18760   1.16360   1.15140   1.12810   1.11610   1.09190   1.07920   1.05250   1.03510

INITIAL RW  PROFILE
   3.43370   3.27700   3.12140   3.13190   2.97060   2.87070   2.89750   2.79580   2.69610   2.71120   2.61370   2.55200
   2.44190   2.36900   2.32130   2.28730   2.21830   2.24740   2.22290   0.00000   2.14020   2.09820   2.06800   2.04960
   2.03790   2.03080   2.02790   2.04140   2.05520   2.07350   2.09510   2.11830   2.16720   2.20920   2.23930   2.24980
   2.23330   2.17910   2.07450   2.04930   1.89950   1.87440   1.75350   1.73200   1.71150   1.59370   1.57580   1.54270
   1.45710   1.42740   1.41220   1.30650   1.29270   1.26660   1.19530   1.16930   1.15570   1.05260   1.03510

DEPS/DXI
   0.0
SPECIES INPUTS
NO. ELEMENTS =      5
```

NUMBER DENSITIES (PARTICLES/CM3)

ETA	N2	O2	N	C	E-	H	C	C2	H2	CC	C3	C2H
0.0	9.67E 15	5.05E 02	2.49E 13	1.95E 10	3.41E 13	1.00E 17	2.91E 15	2.59E 15	1.71E 16	2.80E 16	5.51E 15	1.61E 16
5.00E-03	6.78E 15	7.41E 02	3.32E 13	2.86E 10	3.51E 13	1.03E 17	4.12E 15	3.40E 15	1.33E 16	2.65E 16	6.08E 15	1.48E 16
1.00E-02	7.91E 15	1.11E 03	4.43E 13	4.17E 10	3.13E 13	1.06E 17	5.78E 15	4.38E 15	1.02E 16	2.50E 16	6.51E 15	1.32E 16
1.50E-02	7.07E 15	1.71E 03	5.91E 13	6.18E 10	2.83E 13	1.07E 17	8.04E 15	5.49E 15	7.56E 15	2.36E 16	6.66E 15	1.13E 16
2.00E-02	6.31E 15	2.76E 03	7.91E 13	9.40E 10	3.06E 13	1.07E 17	1.10E 16	6.63E 15	5.48E 15	2.21E 16	6.43E 15	9.18E 15
2.31E-02	5.89E 15	3.84E 03	9.54E 13	1.24E 11	2.97E 13	1.06E 17	1.33E 16	7.30E 15	4.43E 15	2.13E 16	6.06E 15	7.81E 15
2.62E-02	5.52E 15	5.48E 03	1.16E 14	1.67E 11	2.90E 13	1.05E 17	1.59E 16	7.86E 15	3.53E 15	2.04E 16	5.51E 15	6.45E 15
2.94E-02	5.20E 15	8.08E 03	1.41E 14	2.28E 11	2.73E 13	1.04E 17	1.88E 16	8.25E 15	2.79E 15	1.96E 16	4.81E 15	5.15E 15
3.25E-02	4.95E 15	1.24E 04	1.73E 14	3.17E 11	2.66E 13	1.02E 17	2.19E 16	8.41E 15	2.18E 15	1.88E 16	4.01E 15	3.97E 15
3.56E-02	4.76E 15	1.98E 04	2.15E 14	4.52E 11	2.62E 13	1.00E 17	2.52E 16	8.29E 15	1.69E 15	1.81E 16	3.17E 15	2.94E 15
3.87E-02	4.65E 15	3.30E 04	2.69E 14	6.61E 11	2.54E 13	9.76E 16	2.85E 16	7.89E 15	1.29E 15	1.74E 16	2.36E 15	2.08E 15
4.50E-02	4.62E 15	1.07E 05	4.35E 14	1.52E 12	2.34E 13	9.26E 16	3.47E 16	6.35E 15	7.46E 14	1.62E 16	1.09E 15	9.17E 14
5.37E-02	4.89E 15	7.33E 05	8.88E 14	5.66E 12	2.20E 13	8.56E 16	4.07E 16	3.71E 15	3.40E 14	1.48E 16	2.61E 14	2.28E 14
6.25E-02	5.11E 15	5.95E 06	1.78E 15	2.27E 13	2.40E 13	7.93E 16	4.33E 16	1.82E 15	1.59E 14	1.37E 16	4.86E 13	4.86E 13
7.12E-02	4.92E 15	4.82E 07	3.30E 15	8.93E 13	3.06E 13	7.36E 16	4.35E 16	8.32E 14	7.63E 13	1.27E 16	8.35E 12	1.00E 13
8.00E-02	4.15E 15	3.55E 08	5.52E 15	3.28E 14	4.76E 13	6.82E 16	4.25E 16	3.78E 14	3.83E 13	1.16E 16	1.48E 12	2.15E 12
8.50E-02	3.52E 15	9.97E 08	6.97E 15	6.44E 14	6.36E 13	6.53E 16	4.17E 16	2.46E 14	2.64E 13	1.09E 16	5.82E 11	9.41E 11
9.25E-02	2.44E 15	3.90E 09	9.20E 15	1.60E 15	1.02E 14	6.09E 16	4.06E 16	1.31E 14	1.52E 13	9.22E 15	1.42E 11	2.78E 11
1.00E-01	1.48E 15	1.20E 10	1.13E 16	2.99E 15	1.48E 14	5.63E 16	3.98E 16	7.23E 13	8.65E 12	7.13E 15	4.29E 10	8.67E 10
1.10E-01	5.67E 14	2.48E 10	1.25E 16	5.71E 15	2.87E 14	5.06E 16	3.66E 16	3.35E 13	4.17E 12	3.55E 15	8.00E 09	1.90E 10
1.20E-01	2.02E 14	2.40E 10	1.29E 16	7.33E 15	5.39E 14	4.58E 16	3.67E 16	1.57E 13	2.13E 12	1.27E 15	1.57E 09	4.44E 09
1.30E-01	7.84E 13	1.67E 10	1.30E 16	7.71E 15	9.39E 14	4.20E 16	3.40E 16	7.49E 12	1.17E 12	4.16E 14	3.34E 08	1.14E 09
1.40E-01	3.45E 13	1.09E 10	1.32E 16	7.63E 15	1.51E 15	3.87E 16	3.09E 16	3.75E 12	6.95E 11	1.45E 14	8.10E 07	3.35E 08
1.50E-01	1.72E 13	7.32E 09	1.34E 16	7.42E 15	2.25E 15	3.58E 16	2.79E 16	1.98E 12	4.37E 11	5.65E 13	2.24E 07	1.10E 08
1.60E-01	9.59E 12	5.18E 09	1.36E 16	7.21E 15	3.12E 15	3.32E 16	2.49E 16	1.09E 12	2.90E 11	2.46E 13	6.98E 06	4.06E 07
1.70E-01	5.96E 12	3.87E 09	1.40E 16	7.02E 15	4.06E 15	3.08E 16	2.20E 16	6.31E 11	2.01E 11	1.19E 13	2.43E 06	1.65E 07
1.80E-01	4.08E 12	3.04E 09	1.44E 16	6.87E 15	5.00E 15	2.86E 16	1.93E 16	3.79E 11	1.46E 11	6.38E 12	9.32E 05	7.36E 06
2.00E-01	2.45E 12	2.17E 09	1.54E 16	6.72E 15	6.64E 15	2.49E 16	1.48E 16	1.54E 11	8.48E 10	2.35E 12	1.81E 05	1.85E 06
2.10E-01	2.09E 12	1.94E 09	1.61E 16	6.71E 15	7.29E 15	2.33E 16	1.30E 16	1.03E 11	6.73E 10	1.58E 12	8.91E 04	1.02E 06
2.20E-01	1.89E 12	1.80E 09	1.68E 16	6.74E 15	7.81E 15	2.18E 16	1.15E 16	7.16E 10	5.45E 10	1.13E 12	4.73E 04	6.01E 05
2.30E-01	1.78E 12	1.71E 09	1.77E 16	6.81E 15	8.21E 15	2.04E 16	1.01E 16	5.11E 10	4.48E 10	8.54E 11	2.67E 04	3.70E 05
2.40E-01	1.74E 12	1.67E 09	1.87E 16	6.92E 15	8.52E 15	1.90E 16	9.00E 15	3.74E 10	3.72E 10	6.70E 11	1.56E 04	2.37E 05
2.60E-01	1.78E 12	1.67E 09	2.08E 16	7.22E 15	8.90E 15	1.65E 16	7.11E 15	2.09E 10	2.58E 10	4.47E 11	6.05E 03	1.03E 05
2.80E-01	1.85E 12	1.71E 09	2.31E 16	7.57E 15	9.17E 15	1.39E 16	5.51E 15	1.14E 10	1.73E 10	3.04E 11	2.29E 03	4.41E 04
3.00E-01	2.13E 12	1.87E 09	2.57E 16	8.04E 15	9.11E 15	1.16E 16	4.35E 15	6.84E 09	1.17E 10	2.35E 11	1.03E 03	2.11E 04
3.30E-01	2.40E 12	2.04E 09	2.91E 16	8.65E 15	9.14E 15	8.27E 15	2.84E 15	2.71E 09	5.60E 09	1.44E 11	2.43E 02	5.57E 03
3.50E-01	2.40E 12	2.08E 09	3.07E 16	8.92E 15	9.33E 15	6.24E 15	2.00E 15	1.27E 09	3.06E 09	9.35E 10	7.46E 01	1.87E 03
3.80E-01	2.14E 12	1.95E 09	3.18E 16	9.06E 15	9.88E 15	3.69E 15	1.06E 15	3.23E 08	9.99E 08	4.16E 10	8.92E 00	2.56E 02
4.20E-01	1.64E 12	1.74E 09	3.13E 16	8.92E 15	1.09E 16	1.48E 15	3.74E 14	3.50E 07	1.46E 08	1.12E 10	2.92E-01	9.83E 00
4.40E-01	1.42E 12	1.60E 09	3.06E 16	8.76E 15	1.14E 16	8.18E 14	1.96E 14	9.01E 06	4.27E 07	5.12E 09	3.52E-02	1.32E 00
4.80E-01	1.06E 12	1.35E 09	2.88E 16	8.35E 15	1.24E 16	2.10E 14	4.58E 13	4.50E 05	2.62E 06	9.60E 08	3.54E-04	1.56E-02
5.00E-01	9.35E 11	1.26E 09	2.80E 16	8.16E 15	1.28E 16	7.80E 13	1.64E 13	5.59E 04	3.53E 05	3.12E 08	3.91E-05	6.58E-04
5.40E-01	7.52E 11	1.11E 09	2.64E 16	7.81E 15	1.35E 16	1.34E 13	2.65E 12	1.38E 03	9.91E 03	4.36E 07	4.22E-06	7.12E-07
5.60E-01	6.82E 11	1.04E 09	2.57E 16	7.66E 15	1.38E 16	1.32E 13	2.55E 12	1.24E 03	9.50E 03	3.92E 07	4.17E-06	7.03E-07
5.80E-01	6.20E 11	9.83E 08	2.51E 16	7.50E 15	1.41E 16	1.30E 13	2.46E 12	1.13E 03	9.11E 03	3.54E 07	4.13E-06	6.95E-07
6.20E-01	5.10E 11	8.76E 08	2.38E 16	7.22E 15	1.46E 16	1.28E 13	2.29E 12	9.24E 02	8.41E 03	2.88E 07	4.04E-06	6.80E-07
6.40E-01	4.66E 11	8.30E 08	2.32E 16	7.08E 15	1.48E 16	1.26E 13	2.21E 12	8.44E 02	8.09E 03	2.62E 07	3.99E-06	6.73E-07
6.80E-01	3.91E 11	7.45E 08	2.21E 16	6.82E 15	1.53E 16	1.24E 13	2.07E 12	7.06E 02	7.52E 03	2.18E 07	3.91E-06	6.59E-07
7.00E-01	3.63E 11	7.08E 08	2.15E 16	6.68E 15	1.55E 16	1.22E 13	2.00E 12	6.55E 02	7.26E 03	2.01E 07	3.87E-06	6.52E-07
7.40E-01	3.01E 11	6.34E 08	2.05E 16	6.43E 15	1.60E 16	1.20E 13	1.87E 12	5.44E 02	6.75E 03	1.66E 07	3.79E-06	6.39E-07
7.60E-01	2.80E 11	6.03E 08	1.95E 16	6.30E 15	1.62E 16	1.19E 13	1.81E 12	5.05E 02	6.52E 03	1.54E 07	3.75E-06	6.32E-07
8.00E-01	2.32E 11	5.39E 08	1.89E 16	6.05E 15	1.66E 16	1.16E 13	1.69E 12	4.19E 02	6.06E 03	1.27E 07	3.68E-06	6.20E-07
8.20E-01	2.15E 11	5.11E 08	1.84E 16	5.92E 15	1.69E 16	1.15E 13	1.63E 12	3.85E 02	5.85E 03	1.18E 07	3.64E-06	6.13E-07
8.60E-01	1.77E 11	4.55E 08	1.74E 16	5.68E 15	1.73E 16	1.13E 13	1.52E 12	3.21E 02	5.44E 03	9.66E 06	3.57E-06	6.01E-07
8.80E-01	1.64E 11	4.31E 08	1.69E 16	5.55E 15	1.75E 16	1.12E 13	1.47E 12	2.98E 02	5.25E 03	8.93E 06	3.53E-06	5.94E-07
9.20E-01	1.33E 11	3.79E 08	1.58E 16	5.30E 15	1.79E 16	1.09E 13	1.36E 12	2.43E 02	4.85E 03	7.23E 06	3.45E-06	5.82E-07
9.40E-01	1.18E 11	3.52E 08	1.53E 16	5.16E 15	1.81E 16	1.08E 13	1.30E 12	2.16E 02	4.64E 03	6.40E 06	3.41E-06	5.75E-07
9.80E-01	9.51E 10	3.05E 08	1.42E 16	4.87E 15	1.86E 16	1.05E 13	1.19E 12	1.76E 02	4.26E 03	5.19E 06	3.33E-06	5.61E-07
1.00E 00	7.92E 10	2.74E 08	1.35E 16	4.68E 15	1.89E 16	1.04E 13	1.12E 12	1.48E 02	4.00E 03	4.33E 06	3.27E-06	5.51E-07

CONTINUUM CONTRIBUTION TO THE SPECTRAL FLUX

		ETA = 0.0		ETA = 0.500		ETA = 1.000	
I	HNU	QMINUS	QPLUS	QMINUS	QPLUS	QMINUS	QPLUS
1	5.000	0.0	6.212E 01	5.235E-03	1.080E-04	6.213E 01	0.0
2	6.000	0.0	2.742E 00	8.535E-03	1.085E-04	2.802E 00	0.0
3	7.000	0.0	1.647E 00	6.654E-02	1.670E-05	1.666E 00	0.0
4	8.000	0.0	3.153E 00	1.031E-01	2.914E-02	3.457E 00	0.0
5	9.000	0.0	2.917E 00	1.673E-01	2.084E-01	4.413E 00	0.0
6	10.000	0.0	1.783E 00	2.689E-01	3.025E-01	1.943E 00	0.0
7	10.800	0.0	7.986E 00	4.026E-03	5.030E-04	8.806E 00	0.0
8	11.100	0.0	1.995E 01	1.961E-04	5.030E-04	2.381E 01	0.0
9	12.000	0.0	1.576E 01	3.315E-21	1.331E-04	5.376E 01	0.0
10	13.400	0.0	2.887E 01	2.872E-01	1.110E-04	1.369E 02	0.0
11	14.300	0.0	2.614E 00	2.559E-01	1.114E-04	5.529E 01	0.0
12	20.000	0.0	5.394E 00	3.498E 00	1.707E-05	1.040E 02	0.0
TOTAL FLUX		0.0	1.549E 02	4.665E 00	5.416E-01	4.589E 02	0.0

LINE CONTRIBUTION TO THE SPECTRAL FLUX

		ETA = 0.0		ETA = 0.500		ETA = 1.000	
I	HNU	QMINUS	QPLUS	QMINUS	QPLUS	QMINUS	QPLUS
1	1.300	0.0	7.021E 01	0.0	0.0	7.379E 01	0.0
2	2.700	0.0	1.869E 01	0.0	0.0	1.853E 01	0.0
3	5.750	0.0	3.855E 00	0.0	0.0	8.118E 00	0.0
4	7.570	0.0	4.061E 01	0.0	0.0	9.114E 01	0.0
5	9.100	0.0	3.835E 01	0.0	0.0	8.659E 01	0.0
6	10.400	0.0	6.289E 01	0.0	0.0	1.448E 02	0.0
7	11.400	0.0	7.452E 00	0.0	0.0	1.045E 02	0.0
8	12.700	0.0	1.019E-01	0.0	0.0	5.175E 01	0.0
9	13.900	0.0	-3.010E-01	0.0	0.0	3.123E 01	0.0
TOTAL FLUX		0.0	2.419E 02	0.0	0.0	6.105E 02	0.0

SOLUTION CONVERGED IN 3 ITERATIONS


```
XI  =    0.0        DELTA =   3.946145E-02          CTIL =    5.383645E-02

EPS =    0.0        QC =  -0.119654E 03  (WATTS/CM**2)  =  -0.105296E 03  (BTU/FT**2 - SEC)

RD  =    0.0536     QR =  -0.356790E 03  (WATTS/CM**2)  =  -0.349182E 03  (BTU/FT**2 - SEC)

RVW=     0.0500     QKR = -0.296567E 03           CFR =  -0.134537E 03
                    QRT = -0.294698E 03           QT  =  -0.591265E 03        LAMBDA =   -0.491320E-01

TOTAL HEATING  =  -0.516452E 03  (WATTS/CM**2)  =  -0.454478E 03  (BTU/FT**2 - SEC)

HEATING DISTRIBUTION     QC/QCZ =  0.100000E 01   QR/QRZ =  0.100000E 01   QT/QTZ =  0.100000E 01
```

	ETA	Y/DZ	F*	RV	T/TD	E(WATTS/CM3)	V	V (FT/SEC)	G	H (STATIC)
WALL	0.0	0.0	0.0	2.683E-03	2.654E-01	-5.902E 01	5.121E-04	2.561E 01	2.427E-01	2.427E-01
	0.005	1.336E-03	2.737E-03	2.682E-03	2.710E-01	-5.512E 01	5.431E-04	2.715E 01	2.565E-01	2.565E-01
	0.010	2.754E-03	5.699E-03	2.680E-03	2.769E-01	-5.122E 01	5.769E-04	2.885E 01	2.718E-01	2.718E-01
	0.015	4.264E-03	8.816E-03	2.676E-03	2.831E-01	-5.018E 01	6.141E-04	3.070E 01	2.949E-01	2.949E-01
	0.020	5.874E-03	1.210E-02	2.670E-03	2.897E-01	-4.914E 01	6.549E-04	3.275E 01	3.140E-01	3.140E-01
	0.023	6.935E-03	1.430E-02	2.666E-03	2.940E-01	-5.022E 01	6.825E-04	3.412E 01	3.270E-01	3.270E-01
	0.026	8.043E-03	1.657E-02	2.661E-03	2.985E-01	-5.130E 01	7.115E-04	3.558E 01	3.459E-01	3.459E-01
	0.029	9.200E-03	1.891E-02	2.655E-03	3.032E-01	-5.376E 01	7.419E-04	3.710E 01	3.602E-01	3.602E-01
	0.032	1.041E-02	2.139E-02	2.648E-03	3.082E-01	-5.621E 01	7.734E-04	3.867E 01	3.749E-01	3.749E-01
	0.036	1.167E-02	2.394E-02	2.640E-03	3.134E-01	-5.975E 01	8.055E-04	4.028E 01	3.946E-01	3.946E-01
	0.039	1.299E-02	2.658E-02	2.632E-03	3.188E-01	-6.329E 01	8.377E-04	4.189E 01	4.088E-01	4.088E-01
	0.045	1.578E-02	3.221E-02	2.612E-03	3.304E-01	-7.094E 01	8.997E-04	4.498E 01	4.397E-01	4.397E-01
	0.054	2.003E-02	4.060E-02	2.578E-03	3.483E-01	-8.164E 01	9.734E-04	4.867E 01	4.695E-01	4.695E-01
	0.063	2.465E-02	4.957E-02	2.535E-03	3.678E-01	-8.811E 01	1.031E-03	5.155E 01	4.883E-01	4.883E-01
	0.071	2.959E-02	5.906E-02	2.484E-03	3.884E-01	-9.457E 01	1.078E-03	5.390E 01	5.022E-01	5.022E-01
	0.080	3.484E-02	6.903E-02	2.424E-03	4.100E-01	-9.769E 01	1.118E-03	5.590E 01	5.161E-01	5.161E-01
	0.085	3.798E-02	7.493E-02	2.385E-03	4.227E-01	-9.947E 01	1.137E-03	5.686E 01	5.256E-01	5.256E-01
	0.092	4.291E-02	8.408E-02	2.321E-03	4.426E-01	-1.011E 02	1.167E-03	5.834E 01	5.447E-01	5.447E-01
	0.100	4.813E-02	9.356E-02	2.249E-03	4.638E-01	-1.028E 02	1.199E-03	5.993E 01	5.717E-01	5.717E-01
	0.110	5.561E-02	1.068E-01	2.141E-03	4.944E-01	-1.057E 02	1.236E-03	6.179E 01	6.146E-01	6.146E-01
	0.120	6.369E-02	1.206E-01	2.019E-03	5.271E-01	-1.086E 02	1.250E-03	6.251E 01	6.486E-01	6.486E-01
	0.130	7.231E-02	1.348E-01	1.882E-03	5.601E-01	-1.124E 02	1.232E-03	6.159E 01	6.663E-01	6.663E-01
	0.140	8.138E-02	1.493E-01	1.729E-03	5.915E-01	-1.163E 02	1.184E-03	5.922E 01	6.759E-01	6.759E-01
	0.150	9.081E-02	1.639E-01	1.560E-03	6.205E-01	-1.159E 02	1.111E-03	5.555E 01	6.829E-01	6.829E-01
	0.160	1.006E-01	1.786E-01	1.376E-03	6.468E-01	-1.156E 02	1.012E-03	5.060E 01	6.885E-01	6.885E-01
	0.170	1.105E-01	1.934E-01	1.176E-03	6.694E-01	-1.066E 02	8.873E-04	4.437E 01	6.922E-01	6.922E-01
	0.180	1.207E-01	2.081E-01	9.595E-04	6.898E-01	-9.756E 01	7.382E-04	3.691E 01	6.935E-01	6.935E-01
	0.200	1.412E-01	2.368E-01	4.805E-04	7.208E-01	-6.049E 01	3.760E-04	1.880E 01	6.863E-01	6.863E-01
	0.210	1.514E-01	2.503E-01	2.184E-04	7.329E-01	-4.196E 01	1.709E-04	8.544E 00	6.790E-01	6.790E-01
	0.220	1.616E-01	2.632E-01	-5.801E-05	7.432E-01	-2.546E 01	-4.519E-05	-2.259E 00	6.667E-01	6.667E-01
	0.230	1.717E-01	2.753E-01	-3.478E-04	7.521E-01	-8.957E 00	-2.687E-04	-1.343E 01	6.597E-01	6.597E-01
	0.240	1.816E-01	2.868E-01	-6.504E-04	7.601E-01	4.542E 00	-4.969E-04	-2.485E 01	6.466E-01	6.466E-01
	0.260	2.011E-01	3.076E-01	-1.290E-03	7.744E-01	3.154E 01	-9.608E-04	-4.804E 01	6.296E-01	6.296E-01
	0.280	2.201E-01	3.267E-01	-1.973E-03	7.888E-01	4.901E 01	-1.436E-03	-7.181E 01	6.159E-01	6.159E-01
	0.300	2.387E-01	3.448E-01	-2.696E-03	8.021E-01	6.648E 01	-1.890E-03	-9.450E 01	6.066E-01	6.066E-01
	0.330	2.659E-01	3.717E-01	-3.853E-03	8.240E-01	6.300E 01	-2.587E-03	-1.294E 02	6.075E-01	6.075E-01

0.350	2.840E-01	3.901E-01	-4.673E-03	8.382E-01	6.068E 01	-3.094E-03	-1.547E 02	6.145E-01	6.145E-01
0.380	3.111E-01	4.188E-01	-5.979E-03	8.574E-01	6.968E 01	-3.961E-03	-1.981E 02	6.316E-01	6.316E-01
0.420	3.481E-01	4.586E-01	-7.868E-03	8.782E-01	8.168E 01	-5.350E-03	-2.675E 02	6.600E-01	6.600E-01
0.440	3.670E-01	4.784E-01	-8.876E-03	8.867E-01	8.304E 01	-6.138E-03	-3.069E 02	6.725E-01	6.724E-01
0.480	4.057E-01	5.175E-01	-1.102E-02	9.005E-01	8.576E 01	-7.897E-03	-3.948E 02	7.033E-01	7.033E-01
0.500	4.256E-01	5.368E-01	-1.216E-02	9.059E-01	8.912E 01	-8.844E-03	-4.422E 02	7.143E-01	7.142E-01
0.540	4.660E-01	5.749E-01	-1.455E-02	9.149E-01	9.583E 01	-1.088E-02	-5.438E 02	7.384E-01	7.383E-01
0.560	4.866E-01	5.939E-01	-1.581E-02	9.189E-01	1.020E 02	-1.196E-02	-5.982E 02	7.478E-01	7.477E-01
0.580	5.075E-01	6.127E-01	-1.711E-02	9.227E-01	1.082E 02	-1.310E-02	-6.550E 02	7.570E-01	7.569E-01
0.620	5.499E-01	6.504E-01	-1.982E-02	9.302E-01	1.217E 02	-1.553E-02	-7.763E 02	7.792E-01	7.789E-01
0.640	5.715E-01	6.691E-01	-2.124E-02	9.337E-01	1.285E 02	-1.682E-02	-8.412E 02	7.885E-01	7.882E-01
0.680	6.152E-01	7.063E-01	-2.421E-02	9.406E-01	1.434E 02	-1.957E-02	-9.786E 02	8.058E-01	8.054E-01
0.700	6.375E-01	7.249E-01	-2.575E-02	9.441E-01	1.509E 02	-2.104E-02	-1.052E 03	8.191E-01	8.187E-01
0.740	6.826E-01	7.621E-01	-2.895E-02	9.508E-01	1.684E 02	-2.414E-02	-1.207E 03	8.366E-01	8.360E-01
0.760	7.055E-01	7.805E-01	-3.061E-02	9.542E-01	1.771E 02	-2.579E-02	-1.290E 03	8.461E-01	8.454E-01
0.800	7.521E-01	8.175E-01	-3.405E-02	9.609E-01	1.987E 02	-2.928E-02	-1.464E 03	8.690E-01	8.681E-01
0.820	7.757E-01	8.359E-01	-3.583E-02	9.643E-01	2.095E 02	-3.114E-02	-1.557E 03	8.787E-01	8.777E-01
0.860	8.237E-01	8.725E-01	-3.951E-02	9.710E-01	2.379E 02	-3.503E-02	-1.752E 03	8.974E-01	8.961E-01
0.880	8.480E-01	8.909E-01	-4.140E-02	9.746E-01	2.521E 02	-3.711E-02	-1.856E 03	9.117E-01	9.103E-01
0.920	8.975E-01	9.275E-01	-4.532E-02	9.819E-01	2.998E 02	-4.152E-02	-2.076E 03	9.324E-01	9.307E-01
0.940	9.226E-01	9.457E-01	-4.733E-02	9.859E-01	3.237E 02	-4.388E-02	-2.194E 03	9.437E-01	9.417E-01
0.980	9.739E-01	9.822E-01	-5.148E-02	9.942E-01	4.540E 02	-4.893E-02	-2.446E 03	9.739E-01	9.715E-01
SHOC 1.000	1.000E 00	1.000E 00	-5.362E-02	1.000E 00	5.191E 02	-5.181E-02	-2.591E 03	9.907E-01	9.880E-01

-SHOCK LAYER GAS PROPERTIES-

ETA	Y/D	P (ATM.)	T (DEG.KEL.)	RHO (SLUGS/FT3)	MU (LBM/FT-SEC)	RMU (LBF2-SEC3/FT6)	K (BTU/FT-SEC-R)
0.0	0.0	9.8952E-02	3.4500E 03	8.7212E-06	6.2556E-05	1.3527E-11	3.8267E-04
0.0050	1.3361E-03	9.8952E-02	3.5225E 03	8.2250E-06	6.2556E-05	1.2759E-11	3.8267E-04
0.0100	2.7545E-03	9.8952E-02	3.5989E 03	7.7395E-06	6.2556E-05	1.2008E-11	3.8267E-04
0.0150	4.2637E-03	9.8952E-02	3.6796E 03	7.2646E-06	6.6801E-05	1.2039E-11	4.2309E-04
0.0200	5.8737E-03	9.8952E-02	3.7651E 03	6.8022E-06	6.6801E-05	1.1276E-11	4.2309E-04
0.0231	6.9354E-03	9.8952E-02	3.8214E 03	6.5203E-06	6.6801E-05	1.0811E-11	4.2309E-04
0.0262	8.0435E-03	9.8952E-02	3.8802E 03	6.2460E-06	7.0536E-05	1.0939E-11	4.2253E-04
0.0294	9.2004E-03	9.8952E-02	3.9416E 03	5.9811E-06	7.0536E-05	1.0478E-11	4.2253E-04
0.0325	1.0409E-02	9.8952E-02	4.0058E 03	5.7278E-06	7.0536E-05	1.0038E-11	4.2253E-04
0.0356	1.1670E-02	9.8952E-02	4.0731E 03	5.4877E-06	7.4355E-05	1.0141E-11	3.7100E-04
0.0387	1.2985E-02	9.8952E-02	4.1436E 03	5.2641E-06	7.4355E-05	9.7313E-12	3.7100E-04
0.0450	1.5779E-02	9.8952E-02	4.2947E 03	4.8727E-06	7.8774E-05	9.5494E-12	2.8910E-04
0.0537	2.0034E-02	9.8952E-02	4.5275E 03	4.4519E-06	8.3037E-05	9.2034E-12	2.3273E-04
0.0625	2.4648E-02	9.8952E-02	4.7801E 03	4.1396E-06	8.7229E-05	8.9950E-12	2.1251E-04
0.0712	2.9586E-02	9.8952E-02	5.0481E 03	3.8850E-06	9.1444E-05	8.8550E-12	2.1772E-04
0.0800	3.4839E-02	9.8952E-02	5.3287E 03	3.6587E-06	9.5824E-05	8.7427E-12	2.4077E-04
0.0850	3.7983E-02	9.8952E-02	5.4936E 03	3.5372E-06	9.8439E-05	8.6809E-12	2.6805E-04
0.0925	4.2913E-02	9.8952E-02	5.7524E 03	3.3518E-06	1.0268E-04	8.5767E-12	3.1488E-04
0.1000	4.8132E-02	9.8952E-02	6.0284E 03	3.1560E-06	1.0748E-04	8.4464E-12	3.4489E-04
0.1100	5.5609E-02	9.8952E-02	6.4263E 03	2.9054E-06	1.1430E-04	8.2583E-12	3.3272E-04
0.1200	6.3692E-02	9.8952E-02	6.8516E 03	2.6999E-06	1.2088E-04	8.1066E-12	2.7099E-04
0.1300	7.2314E-02	9.8952E-02	7.2800E 03	2.5519E-06	1.2640E-04	8.0098E-12	2.4735E-04
0.1400	8.1379E-02	9.8952E-02	7.6885E 03	2.4416E-06	1.3068E-04	7.9269E-12	2.5767E-04
0.1500	9.0813E-02	9.8952E-02	8.0658E 03	2.3560E-06	1.3375E-04	7.8386E-12	2.8295E-04
0.1600	1.0055E-01	9.8952E-02	8.4065E 03	2.2903E-06	1.3581E-04	7.7503E-12	3.1451E-04
0.1700	1.1053E-01	9.8952E-02	8.7066E 03	2.2430E-06	1.3711E-04	7.6790E-12	3.4726E-04
0.1800	1.2069E-01	9.8952E-02	8.9666E 03	2.2126E-06	1.3798E-04	7.6408E-12	3.7753E-04
0.2000	1.4119E-01	9.8952E-02	9.3666E 03	2.2009E-06	1.3951E-04	7.7210E-12	4.2441E-04
0.2100	1.5145E-01	9.8952E-02	9.5263E 03	2.2122E-06	1.4037E-04	7.8249E-12	4.4250E-04
0.2200	1.6162E-01	9.8952E-02	9.6602E 03	2.2328E-06	1.4037E-04	7.9124E-12	4.4250E-04
0.2300	1.7170E-01	9.8952E-02	9.7763E 03	2.2599E-06	1.4243E-04	8.1378E-12	4.7200E-04
0.2400	1.8164E-01	9.8952E-02	9.8799E 03	2.2910E-06	1.4243E-04	8.2588E-12	4.7200E-04
0.2600	2.0111E-01	9.8952E-02	1.0065E 04	2.3568E-06	1.4568E-04	8.6995E-12	5.1623E-04
0.2800	2.2010E-01	9.8952E-02	1.0253E 04	2.4104E-06	1.4719E-04	8.9885E-12	5.5904E-04
0.3000	2.3865E-01	9.8952E-02	1.0425E 04	2.4670E-06	1.4812E-04	9.2048E-12	6.1000E-04
0.3300	2.6593E-01	9.8952E-02	1.0711E 04	2.5091E-06	1.4745E-04	9.2194E-12	7.1500E-04
0.3500	2.8395E-01	9.8952E-02	1.0895E 04	2.5115E-06	1.4595E-04	9.0847E-12	7.9213E-04
0.3800	3.1113E-01	9.8952E-02	1.1144E 04	2.4838E-06	1.4270E-04	8.7442E-12	9.0560E-04
0.4200	3.4809E-01	9.8952E-02	1.1415E 04	2.4138E-06	1.3768E-04	8.1896E-12	1.0349E-03
0.4400	3.6698E-01	9.8952E-02	1.1526E 04	2.3749E-06	1.3768E-04	8.0594E-12	1.0349E-03
0.4800	4.0573E-01	9.8952E-02	1.1704E 04	2.2979E-06	1.3073E-04	7.4129E-12	1.1640E-03
0.5000	4.2556E-01	9.8952E-02	1.1775E 04	2.2653E-06	1.3073E-04	7.3107E-12	1.1640E-03
0.5400	4.6602E-01	9.8952E-02	1.1892E 04	2.2077E-06	1.2558E-04	6.8484E-12	1.2379E-03
0.5600	4.8664E-01	9.8952E-02	1.1944E 04	2.1817E-06	1.2558E-04	6.7694E-12	1.2379E-03
0.5800	5.0750E-01	9.8952E-02	1.1994E 04	2.1571E-06	1.2558E-04	6.6938E-12	1.2379E-03
0.6200	5.4991E-01	9.8952E-02	1.2091E 04	2.1106E-06	1.1996E-04	6.2586E-12	1.3176E-03
0.6400	5.7146E-01	9.8952E-02	1.2137E 04	2.0879E-06	1.1996E-04	6.1918E-12	1.3176E-03
0.6800	6.1525E-01	9.8952E-02	1.2226E 04	2.0459E-06	1.1996E-04	6.0686E-12	1.3176E-03
0.7000	6.3748E-01	9.8952E-02	1.2271E 04	2.0243E-06	1.1469E-04	5.7413E-12	1.3551E-03
0.7400	6.8263E-01	9.8952E-02	1.2359E 04	1.9847E-06	1.1469E-04	5.6297E-12	1.3551E-03
0.7600	7.0555E-01	9.8952E-02	1.2402E 04	1.9642E-06	1.1469E-04	5.5718E-12	1.3551E-03
0.8000	7.5208E-01	9.8952E-02	1.2490E 04	1.9257E-06	1.0854E-04	5.1706E-12	1.4100E-03
0.8200	7.7569E-01	9.8952E-02	1.2533E 04	1.9059E-06	1.0854E-04	5.1179E-12	1.4100E-03
0.8600	8.2365E-01	9.8952E-02	1.2622E 04	1.8682E-06	1.0854E-04	5.0175E-12	1.4100E-03
0.8800	8.4800E-01	9.8952E-02	1.2667E 04	1.8485E-06	1.0359E-04	4.7380E-12	1.4199E-03
0.9200	8.9746E-01	9.8952E-02	1.2763E 04	1.8092E-06	1.0359E-04	4.6381E-12	1.4199E-03
0.9400	9.2263E-01	9.8952E-02	1.2814E 04	1.7884E-06	1.0359E-04	4.5850E-12	1.4199E-03
0.9800	9.7386E-01	9.8952E-02	1.2922E 04	1.7452E-06	9.6925E-05	4.1874E-12	1.4283E-03
1.0000	1.0000E 00	9.8952E-02	1.2998E 04	1.7165E-06	9.6925E-05	4.1185E-12	1.4283E-03

-SPECIES MASS FRACTIONS-

	C2	N2	C	N	O+	N+	E-
0.0	4.8110E-15	5.3703E-02	9.7359E-08	9.4364E-05	1.6573E-20	5.7159E-18	1.1314E-09
0.0050	7.3839E-15	5.1156E-02	1.5970E-07	1.3280E-04	2.8218E-20	1.3441E-17	2.1749E-09
0.0100	1.1607E-14	4.8352E-02	2.4597E-07	1.8692E-04	4.9059E-19	1.2624E-16	3.3392E-09
0.0150	1.8855E-14	4.5496E-02	3.8634E-07	2.6386E-04	2.3591E-18	4.1715E-16	3.0655E-09
0.0200	3.2011E-14	4.2861E-02	6.2240E-07	3.7479E-04	1.1942E-17	2.8704E-15	2.8928E-09
0.0231	4.5879E-14	4.1461E-02	8.5259E-07	4.6941E-04	2.2395E-17	5.2652E-15	4.1721E-09
0.0262	6.7580E-14	4.0359E-02	1.1861E-06	5.9160E-04	5.7082E-17	7.2221E-15	3.8580E-09
0.0294	1.0270E-13	3.9648E-02	1.6782E-06	7.5115E-04	1.7987E-16	1.2808E-14	4.0366E-09
0.0325	1.6176E-13	3.9431E-02	2.4208E-06	9.6228E-04	5.3856E-16	1.0175E-13	4.1105E-09
0.0356	2.6560E-13	3.9814E-02	3.5704E-06	1.2461E-03	1.1370E-15	2.6642E-13	4.3428E-09
0.0387	4.5618E-13	4.0907E-02	5.3899E-06	1.6316E-03	2.0150E-15	6.9529E-13	4.7269E-09
0.0450	1.5510E-12	4.5545E-02	1.3192E-05	2.8850E-03	4.6768E-14	5.6237E-12	4.7745E-09
0.0537	1.1287E-11	5.7248E-02	5.2489E-05	6.6316E-03	1.2864E-12	7.4431E-11	5.4184E-09
0.0625	9.6795E-11	7.0820E-02	2.2285E-04	1.4753E-02	2.9941E-11	1.4547E-09	7.2811E-09
0.0712	8.3933E-10	7.9228E-02	9.3031E-04	3.0099E-02	5.4085E-10	1.4506E-08	1.1188E-08
0.0800	6.5205E-09	7.7234E-02	3.5971E-03	5.5072E-02	6.9197E-09	9.7814E-08	2.0264E-08
0.0850	1.9711E-08	7.0910E-02	7.4518E-03	7.3718E-02	2.6223E-08	2.5510E-07	2.9042E-08
0.0925	8.7887E-08	5.5671E-02	2.0363E-02	1.0645E-01	1.7193E-07	9.6502E-07	4.9859E-08
0.1000	3.1494E-07	3.9158E-02	4.2220E-02	1.4572E-01	8.1270E-07	2.7933E-06	7.6269E-08
0.1100	8.1804E-07	1.8157E-02	9.4512E-02	1.8491E-01	5.1888E-06	1.1259E-05	1.6176E-07
0.1200	9.4479E-07	7.6614E-03	1.3775E-01	2.1560E-01	2.0274E-05	3.8845E-05	3.2861E-07
0.1300	7.3068E-07	3.4364E-03	1.5779E-01	2.4216E-01	5.5900E-05	1.1579E-04	6.0581E-07
0.1400	5.2169E-07	1.7521E-03	1.6625E-01	2.6813E-01	1.1266E-04	2.9735E-04	1.0055E-06
0.1500	3.8362E-07	1.0191E-03	1.7090E-01	2.9487E-01	2.5561E-04	6.6205E-04	1.5169E-06
0.1600	2.9703E-07	6.6618E-04	1.7438E-01	3.2260E-01	4.5460E-04	1.3286E-03	2.1039E-06
0.1700	2.4266E-07	4.8246E-04	1.7746E-01	3.5115E-01	7.3798E-04	2.3666E-03	2.7091E-06
0.1800	2.0771E-07	3.7971E-04	1.8038E-01	3.8004E-01	1.1093E-03	3.9397E-03	3.2794E-06
0.2000	1.7154E-07	2.8859E-04	1.8594E-01	4.3762E-01	2.0694E-03	8.5246E-03	4.1326E-06
0.2100	1.6191E-07	2.6679E-04	1.8849E-01	4.6470E-01	2.6450E-03	1.1568E-02	4.4153E-06
0.2200	1.5560E-07	2.5330E-04	1.9089E-01	4.9027E-01	3.2535E-03	1.5042E-02	4.6048E-06
0.2300	1.5138E-07	2.4449E-04	1.9306E-01	5.1402E-01	3.9284E-03	1.8924E-02	4.7266E-06
0.2400	1.4833E-07	2.3765E-04	1.9506E-01	5.3568E-01	4.6120E-03	2.3226E-02	4.7995E-06
0.2600	1.4334E-07	2.2457E-04	1.9827E-01	5.7224E-01	6.2084E-03	3.3179E-02	4.8780E-06
0.2800	1.3620E-07	2.0289E-04	2.0030E-01	5.9866E-01	8.2090E-03	4.5937E-02	5.0119E-06
0.3000	1.2899E-07	1.8116E-04	2.0139E-01	6.1653E-01	1.0444E-02	6.0325E-02	5.1650E-06
0.3300	1.1339E-07	1.3883E-04	2.0096E-01	6.2614E-01	1.4686E-02	8.7667E-02	5.6937E-06
0.3500	1.0294E-07	1.1444E-04	1.9971E-01	6.2451E-01	1.7848E-02	1.0788E-01	6.1708E-06
0.3800	8.8844E-08	8.5518E-05	1.9697E-01	6.1442E-01	2.2650E-02	1.3805E-01	6.9959E-06
0.4200	7.4146E-08	6.0323E-05	1.9268E-01	5.9414E-01	2.8517E-02	1.7365E-01	8.1434E-06
0.4400	6.8216E-08	5.1747E-05	1.9051E-01	5.8316E-01	3.1144E-02	1.8908E-01	8.6977E-06
0.4800	5.9376E-08	3.9806E-05	1.8641E-01	5.6198E-01	3.5657E-02	2.1429E-01	9.7089E-06
0.5000	5.5959E-08	3.5742E-05	1.8462E-01	5.5272E-01	3.7532E-02	2.2445E-01	1.0141E-05
0.5400	5.0573E-08	2.9683E-05	1.8141E-01	5.3605E-01	4.0794E-02	2.4159E-01	1.0908E-05
0.5600	4.8285E-08	2.7288E-05	1.7991E-01	5.2834E-01	4.2295E-02	2.4931E-01	1.1265E-05
0.5800	4.6151E-08	2.5150E-05	1.7842E-01	5.2078E-01	4.3786E-02	2.5686E-01	1.1613E-05
0.6200	4.2116E-08	2.1212E-05	1.7553E-01	5.0618E-01	4.6674E-02	2.7147E-01	1.2286E-05
0.6400	4.0463E-08	1.9869E-05	1.7394E-01	4.9864E-01	4.8257E-02	2.7901E-01	1.2637E-05
0.6800	3.7044E-08	1.6864E-05	1.7108E-01	4.8461E-01	5.1116E-02	2.9304E-01	1.3285E-05
0.7000	3.5612E-08	1.5842E-05	1.6944E-01	4.7708E-01	5.2766E-02	3.0057E-01	1.3639E-05
0.7400	3.2588E-08	1.3454E-05	1.6648E-01	4.6304E-01	5.5723E-02	3.1461E-01	1.4290E-05
0.7600	3.1319E-08	1.2645E-05	1.6476E-01	4.5546E-01	5.7451E-02	3.2219E-01	1.4647E-05
0.8000	2.8582E-08	1.0704E-05	1.6163E-01	4.4112E-01	6.0582E-02	3.3653E-01	1.5317E-05
0.8200	2.7446E-08	1.0057E-05	1.5983E-01	4.3350E-01	6.2391E-02	3.4414E-01	1.5679E-05
0.8600	2.4951E-08	8.4701E-06	1.5649E-01	4.1874E-01	6.5740E-02	3.5889E-01	1.6372E-05
0.8800	2.3881E-08	7.9216E-06	1.5453E-01	4.1076E-01	6.7707E-02	3.6686E-01	1.6752E-05
0.9200	2.1488E-08	6.5767E-06	1.5071E-01	3.9463E-01	7.1539E-02	3.8299E-01	1.7516E-05
0.9400	2.0221E-08	5.8997E-06	1.4861E-01	3.8585E-01	7.3636E-02	3.9176E-01	1.7933E-05
0.9800	1.8004E-08	4.8813E-06	1.4381E-01	3.6725E-01	7.8447E-02	4.1036E-01	1.8826E-05
1.0000	1.6495E-08	4.2239E-06	1.4051E-01	3.5440E-01	8.1751E-02	4.2320E-01	1.9443E-05

-SPECIES MASS FRACTIONS-

ETA	C	H	H2	CO	C3-G	CN	C2H	C2H2
0.0	1.3355E-02	3.8628E-02	1.3630E-02	2.6898E-01	8.1654E-02	7.7916E-02	1.6518E-01	1.6737E-02
0.0500	2.0124E-02	4.2237E-02	1.1259E-02	2.6920E-01	9.6425E-02	8.9449E-02	1.6232E-01	1.2200E-02
0.1000	3.0151E-02	4.5797E-02	9.1136E-03	2.6944E-01	1.1071E-01	1.0148E-01	1.5478E-01	6.5185E-03
0.1500	4.4806E-02	4.9263E-02	7.2131E-03	2.6970E-01	1.2214E-01	1.1354E-01	1.4209E-01	5.6484E-03
0.2000	6.5743E-02	5.2557E-02	5.5810E-03	2.7000E-01	1.2759E-01	1.2506E-01	1.2427E-01	3.5179E-03
0.2312	8.2861E-02	5.4493E-02	4.6965E-03	2.7021E-01	1.2651E-01	1.3170E-01	1.1087E-01	2.5177E-03
0.2625	1.0357E-01	5.6299E-02	3.9068E-03	2.7044E-01	1.2128E-01	1.3772E-01	9.6194E-02	1.7406E-03
0.2937	1.2810E-01	5.7936E-02	3.2196E-03	2.7068E-01	1.1175E-01	1.4291E-01	8.0847E-02	1.1580E-03
0.3250	1.5642E-01	5.9377E-02	2.6275E-03	2.7094E-01	9.8357E-02	1.4709E-01	6.5548E-02	7.3852E-04
0.3562	1.8820E-01	6.0608E-02	2.1133E-03	2.7122E-01	8.2116E-02	1.5003E-01	5.1027E-02	4.4922E-04
0.3875	2.2248E-01	6.1594E-02	1.6918E-03	2.7154E-01	6.4660E-02	1.5152E-01	3.8012E-02	2.6002E-04
0.4500	2.9267E-01	6.2877E-02	1.0508E-03	2.7221E-01	3.3177E-02	1.4927E-01	1.8390E-02	7.5054E-05
0.5375	3.7461E-01	6.3414E-02	5.2727E-04	2.7329E-01	8.6567E-03	1.3358E-01	5.0918E-03	1.0044E-05
0.6250	4.2557E-01	6.3118E-02	2.6740E-04	2.7433E-01	1.8009E-03	1.0760E-01	1.1866E-03	1.1592E-06
0.7125	4.5281E-01	6.2448E-02	1.3974E-04	2.7461E-01	3.3619E-04	7.9377E-02	2.6605E-04	1.3365E-07
0.8000	4.6649E-01	6.1576E-02	7.5076E-05	2.7165E-01	6.3918E-05	5.4423E-02	6.1583E-05	1.6563E-08
0.8500	4.7145E-01	6.1005E-02	5.3514E-05	2.6598E-01	2.5552E-05	4.2605E-02	2.7541E-05	5.2746E-09
0.9250	4.7970E-01	6.0055E-02	3.2565E-05	2.4512E-01	6.7527E-06	2.8177E-02	8.5105E-06	9.9070E-10
1.0000	4.9553E-01	5.8981E-02	1.9558E-05	2.0883E-01	1.9475E-06	6.0546E-03	2.7393E-06	1.9300E-10
1.1000	5.1736E-01	5.7329E-02	1.0194E-05	1.2027E-01	3.9182E-07	3.1280E-03	6.3457E-07	2.3625E-11
1.2000	5.2656E-01	5.5395E-02	5.4643E-06	4.8028E-02	7.9836E-08	1.5373E-03	1.5396E-07	3.1457E-12
1.3000	5.1251E-01	5.3196E-02	3.1062E-06	1.6840E-02	1.7488E-08	7.7627E-04	4.0722E-08	4.9072E-13
1.4000	4.8444E-01	5.0768E-02	1.8769E-06	6.3107E-03	4.2958E-09	4.2409E-04	1.2309E-08	9.4086E-14
1.5000	4.4904E-01	4.8139E-02	1.2287E-06	2.6681E-03	1.2917E-09	2.5211E-04	4.2572E-09	2.2184E-14
1.6000	4.0955E-01	4.5338E-02	8.3343E-07	1.2723E-03	4.3101E-10	1.6154E-04	1.6539E-09	6.1965E-15
1.7000	3.6826E-01	4.2398E-02	5.8818E-07	6.7698E-04	1.6137E-10	1.1051E-04	7.1091E-10	2.0082E-15
1.8000	3.2716E-01	3.9362E-02	4.2440E-07	3.9481E-04	6.6458E-11	7.9668E-05	3.3146E-10	7.3360E-16
2.0000	2.5109E-01	3.3153E-02	2.4214E-07	1.6987E-04	1.4502E-11	4.7416E-05	8.9304E-11	1.3286E-16
2.1000	2.1783E-01	3.0142E-02	1.8575E-07	1.2020E-04	7.3445E-12	3.8022E-05	4.9501E-11	6.2104E-17
2.2000	1.8805E-01	2.7236E-02	1.4265E-07	8.8290E-05	3.8705E-12	3.1040E-05	2.6309E-11	3.0328E-17
2.3000	1.6159E-01	2.4474E-02	1.1074E-07	6.6552E-05	2.0956E-12	2.5610E-05	1.6508E-11	1.5218E-17
2.4000	1.3822E-01	2.1877E-02	8.5286E-08	5.0932E-05	1.1480E-12	2.1202E-05	9.7013E-12	7.7205E-18
2.6000	9.9656E-02	1.7223E-02	5.0035E-08	3.0363E-05	3.4468E-13	1.4422E-05	3.3252E-12	1.9696E-18
2.8000	6.9954E-02	1.3306E-02	2.8061E-08	1.7477E-05	9.4731E-14	9.3141E-06	1.0501E-12	4.4965E-19
3.0000	4.8340E-02	1.0081E-02	1.5152E-08	1.0080E-05	2.5429E-14	5.9034E-06	3.2074E-13	9.8880E-20
3.3000	2.6435E-02	6.3873E-03	5.4432E-09	4.0034E-06	2.8628E-15	2.6680E-06	4.4528E-14	7.3761E-21
3.5000	1.7094E-02	4.5299E-03	2.5382E-09	2.1029E-06	6.1207E-16	1.5052E-06	1.0713E-14	8.3776E-22
3.8000	8.4331E-03	2.5242E-03	7.0431E-10	7.7791E-07	5.2829E-17	6.0664E-07	1.0848E-15	9.6164E-23
4.2000	2.9170E-03	9.9270E-04	9.5558E-11	1.9570E-07	1.5216E-18	1.6517E-07	3.6702E-17	1.1089E-23
4.4000	1.5306E-03	5.4889E-04	2.7606E-11	8.9546E-08	1.8112E-19	7.7861E-08	4.6277E-18	1.2682E-24
4.8000	3.7663E-04	1.4694E-04	1.7964E-12	1.7779E-08	2.0804E-21	1.6065E-08	6.2439E-20	1.4399E-25
5.0000	1.4090E-04	5.6838E-05	2.5651E-13	6.0959E-09	2.3204E-22	5.5874E-09	4.3207E-21	1.6060E-26
5.4000	2.4231E-05	1.0344E-05	7.4234E-15	9.0485E-10	2.5665E-23	8.4781E-10	4.7790E-22	1.7763E-27
5.6000	2.3626E-05	1.0344E-05	7.7714E-15	8.2641E-10	2.5664E-23	7.8111E-10	4.7786E-22	1.7763E-27
5.8000	2.3049E-05	1.0344E-05	7.5500E-15	7.5700E-10	2.5663E-23	7.2148E-10	4.7786E-22	1.7762E-27
6.2000	2.1948E-05	1.0343E-05	7.1277E-15	6.3025E-10	2.5662E-23	6.1150E-10	4.7784E-22	1.7761E-27
6.4000	2.1452E-05	1.0343E-05	6.9514E-15	5.8886E-10	2.5661E-23	5.7361E-10	4.7782E-22	1.7760E-27
6.8000	2.0469E-05	1.0343E-05	6.5672E-15	4.9468E-10	2.5660E-23	4.8957E-10	4.7780E-22	1.7760E-27
7.0000	2.0014E-05	1.0343E-05	6.4308E-15	4.6400E-10	2.5659E-23	4.6075E-10	4.7777E-22	1.7759E-27
7.4000	1.9099E-05	1.0343E-05	6.1026E-15	3.9095E-10	2.5658E-23	3.9353E-10	4.7776E-22	1.7758E-27
7.6000	1.8672E-05	1.0342E-05	5.9607E-15	3.6712E-10	2.5657E-23	3.7061E-10	4.7774E-22	1.7758E-27
8.0000	1.7800E-05	1.0342E-05	5.6559E-15	3.0898E-10	2.5656E-23	3.1577E-10	4.7772E-22	1.7757E-27
8.2000	1.7395E-05	1.0342E-05	5.5255E-15	2.9020E-10	2.5655E-23	2.9731E-10	4.7771E-22	1.7756E-27
8.6000	1.6557E-05	1.0342E-05	5.2410E-15	2.4353E-10	2.5654E-23	2.5228E-10	4.7768E-22	1.7755E-27
8.8000	1.6156E-05	1.0342E-05	5.1139E-15	2.2780E-10	2.5652E-23	2.3653E-10	4.7766E-22	1.7755E-27
9.2000	1.5301E-05	1.0342E-05	4.8318E-15	1.8888E-10	2.5652E-23	1.9812E-10	4.7765E-22	1.7754E-27
9.4000	1.4844E-05	1.0342E-05	4.6812E-15	1.6944E-10	2.5651E-23	1.7872E-10	4.7763E-22	1.7753E-27
9.8000	1.3963E-05	1.0341E-05	4.4058E-15	1.4047E-10	2.5650E-23	1.4931E-10	4.7762E-22	1.7753E-27
10.0000	1.3355E-05	1.0341E-05	4.2144E-15	1.2187E-10	2.5649E-23	1.3020E-10	4.7760E-22	1.7752E-27

-SPECIES MASS FRACTIONS-

ETA	CP	C3H	C4H	HCN	C2	C+	AMW
0.0	6.0950E 00	1.3016E-01	8.4212E-02	1.1046E-02	2.4706E-02	1.4318E-11	1.2881E 01
0.0500	6.3289E 00	1.1452E-01	7.0180E-02	2.6229E-02	3.4577E-02	1.2246E-11	1.2405E 01
0.1000	6.5821E 00	9.6704E-02	5.5544E-02	2.1609E-02	4.7611E-02	1.3096E-10	1.1928E 01
0.1500	6.9703E 00	7.7417E-02	4.1067E-02	1.7313E-02	6.4040E-02	9.4387E-10	1.1450E 01
0.2000	7.2726E 00	5.7859E-02	2.7789E-02	1.3455E-02	8.3347E-02	3.2759E-09	1.0974E 01
0.2312	7.4735E 00	4.6165E-02	2.0570E-02	1.1299E-02	9.6172E-02	5.7085E-09	1.0679E 01
0.2625	7.0356E 00	3.5379E-02	1.4450E-02	9.3564E-03	1.0872E-01	1.3792E-08	1.0396E 01
0.2937	7.2305E 00	2.5894E-02	9.5617E-03	7.6372E-03	1.1990E-01	2.8704E-08	1.0110E 01
0.3250	7.4268E 00	1.7988E-02	5.9112E-03	6.1413E-03	1.2847E-01	6.1184E-08	9.8426E 00
0.3562	5.9562E 00	1.1777E-02	3.3822E-03	4.8610E-03	1.3315E-01	1.3328E-07	9.5918E 00
0.3875	6.1013E 00	7.2325E-03	1.7799E-03	3.7867E-03	1.3291E-01	2.6783E-07	9.3635E 00
0.4500	4.0906E 00	2.2318E-03	3.7895E-04	2.1917E-03	1.1703E-01	7.0954E-07	8.9894E 00
0.5375	2.7153E 00	2.9142E-04	2.6048E-05	9.2597E-04	7.5438E-02	6.8666E-06	8.6644E 00
0.6250	2.1119E 00	2.9711E-05	1.2919E-06	3.6027E-04	3.9911E-02	3.4500E-05	8.5110E 00
0.7125	2.0286E 00	2.8903E-06	6.0278E-08	1.3316E-04	1.9499E-02	1.1758E-04	8.4404E 00
0.8000	2.2636E 00	2.9798E-07	1.7741E-09	4.7561E-05	9.4058E-03	2.9899E-04	8.3945E 00
0.8500	2.6283E 00	8.5591E-08	5.8836E-10	2.6109E-05	6.2715E-03	4.7587E-04	8.3648E 00
0.9250	3.2314E 00	1.3879E-08	5.3727E-11	1.0246E-05	3.4820E-03	9.2476E-04	8.2960E 00
1.0000	3.5329E 00	2.1469E-09	2.7311E-12	3.9382E-06	1.9950E-03	1.4847E-03	8.1798E 00
1.1000	3.1121E 00	2.5225E-10	2.4875E-13	9.6192E-07	9.6277E-04	3.3208E-03	8.0169E 00
1.2000	2.0291E 00	2.8604E-11	1.6214E-14	2.3336E-07	4.8564E-04	6.9120E-03	7.9337E 00
1.3000	1.5628E 00	3.7094E-12	1.1305E-15	6.2755E-08	2.4114E-04	1.2864E-02	7.9652E 00
1.4000	1.5696E 00	5.6934E-13	1.0417E-16	1.9817E-08	1.2534E-04	2.1380E-02	8.0527E 00
1.5000	1.7534E 00	1.1880E-13	1.2666E-17	7.3211E-09	6.8784E-05	3.2132E-02	8.1618E 00
1.6000	1.9932E 00	2.8182E-14	1.9574E-18	3.1000E-09	3.9642E-05	4.4215E-02	8.2836E 00
1.7000	2.2302E 00	7.8177E-15	3.7107E-19	1.4782E-09	2.3848E-05	5.6330E-02	8.4196E 00
1.8000	2.4294E 00	2.4686E-15	8.4247E-20	7.7663E-10	1.4841E-05	6.7143E-02	8.5733E 00
2.0000	2.6766E 00	3.4423E-16	6.9606E-21	2.7489E-10	6.3484E-06	8.1090E-02	8.9527E 00
2.1000	2.7442E 00	1.4326E-16	1.3185E-21	1.7645E-10	4.2762E-06	8.4197E-02	9.1695E 00
2.2000	2.6762E 00	6.2864E-17	1.1947E-22	1.1742E-10	2.9230E-06	8.4873E-02	9.4023E 00
2.3000	2.8136E 00	2.8579E-17	1.1097E-23	7.9929E-11	2.0156E-06	8.3663E-02	9.6447E 00
2.4000	2.7433E 00	1.3194E-17	1.0568E-24	5.4938E-11	1.3932E-06	8.1018E-02	9.8918E 00
2.6000	2.8893E 00	2.8056E-18	1.0318E-25	2.5849E-11	6.5898E-07	7.2950E-02	1.0378E 01
2.8000	3.0025E 00	5.2941E-19	1.0562E-26	1.1201E-11	2.9410E-07	6.3392E-02	1.0811E 01
3.0000	3.1516E 00	9.9135E-20	1.1252E-27	4.7039E-12	1.2841E-07	5.2686E-02	1.1187E 01
3.3000	3.5038E 00	5.3013E-21	1.2390E-28	1.0496E-12	3.2604E-08	3.7578E-02	1.1563E 01
3.5000	3.7672E 00	6.0195E-22	1.4068E-29	3.5195E-13	1.2231E-08	2.8306E-02	1.1709E 01
3.8000	4.1619E 00	6.9095E-23	1.6149E-30	6.1213E-14	2.5582E-09	1.6865E-02	1.1791E 01
4.2000	4.6299E 00	7.9679E-24	1.8622E-31	4.8410E-15	2.5817E-10	7.0326E-03	1.1724E 01
4.4000	4.6595E 00	9.1125E-25	2.1297E-32	1.0955E-15	6.6012E-11	1.9706E-03	1.1650E 01
4.8000	5.1339E 00	1.0346E-25	2.4180E-33	4.8892E-17	3.5570E-12	1.0960E-03	1.1460E 01
5.0000	5.1747E 00	1.1539E-26	2.6969E-34	6.0020E-18	4.7465E-13	4.2878E-04	1.1369E 01
5.4000	5.4525E 00	1.2763E-27	2.9830E-35	1.4047E-19	1.2955E-14	7.9442E-05	1.1194E 01
5.6000	5.4922E 00	1.2763E-27	2.9828E-35	1.0191E-19	1.1881E-14	8.0046E-05	1.1117E 01
5.8000	5.5310E 00	1.2762E-27	2.9827E-35	9.3350E-20	1.0928E-14	8.0621E-05	1.1039E 01
6.2000	5.8168E 00	1.2762E-27	2.9826E-35	4.8205E-20	9.1762E-15	8.1720E-05	1.0891E 01
6.4000	5.8573E 00	1.2761E-27	2.9825E-35	4.8203E-20	8.5923E-15	8.2213E-05	1.0816E 01
6.8000	5.9322E 00	1.2761E-27	2.9824E-35	4.8202E-20	7.2724E-15	8.3193E-05	1.0679E 01
7.0000	5.9980E 00	1.2760E-27	2.9822E-35	2.1438E-20	6.8335E-15	8.3646E-05	1.0606E 01
7.4000	6.0736E 00	1.2760E-27	2.9821E-35	2.1437E-20	5.7969E-15	8.4559E-05	1.0474E 01
7.6000	6.1149E 00	1.2759E-27	2.9820E-35	2.1436E-20	5.4528E-15	8.4983E-05	1.0404E 01
8.0000	6.2664E 00	1.2759E-27	2.9819E-35	2.1435E-20	4.6190E-15	8.5853E-05	1.0273E 01
8.2000	6.3088E 00	1.2758E-27	2.9818E-35	2.1434E-20	4.3455E-15	8.6255E-05	1.0204E 01
8.6000	6.3900E 00	1.2758E-27	2.9816E-35	2.1433E-20	3.6698E-15	8.7089E-05	1.0074E 01
8.8000	6.3295E 00	1.2757E-27	2.9815E-35	2.1432E-20	3.4388E-15	8.7487E-05	1.0004E 01
9.2000	6.4177E 00	1.2757E-27	2.9814E-35	2.1432E-20	2.8702E-15	8.8339E-05	9.8667E 00
9.4000	6.4657E 00	1.2756E-27	2.9813E-35	2.1432E-22	2.5852E-15	8.8795E-05	9.7934E 00
9.8000	6.3927E 00	1.2756E-27	2.9812E-35	2.1431E-22	2.1576E-15	8.9675E-05	9.6396E 00
10.0000	6.4620E 00	1.2755E-27	2.9811E-35	2.1430E-22	1.8810E-15	9.0281E-05	9.5363E 00

APPENDIX G

COMPUTER PROGRAM FOR MULTICOMPONENT DIFFUSION ANALYSIS

The program (SLAM) presented in this appendix consists of the interative numerical solution of the elemental continuity equations (Eqs. 3.97) with offective multicomponent diffusion coefficients as determined by the Stefan-Maxwell Equations (Eqs. 3.98) and equilibrium compositions. A general description of the overall logic and the details of the numerical solutions is given in Chapter V.

A brief description of each of the subprograms included in this code is presented in Table G-1. In the following section, a detailed input guide is given. A complete listing will then follow which includes a sample data package and the corresponding final solution.

Input Guide

The following chart shows the format of the card input.

Card	Variables	Format
1	TITLE	20A4
2	NDBUG, NETA, NSP, NE	3I5, 5X, I5
3	TOL, UINF, DTIL, RAD, RINF, RZB, DELTA	8E10.4
4	ET(N)	6E12.8
5	YOND(N)	6E12.8
6	TT(N)	6E12.8
7	PI(N)	6E12.8
8	VV(N)	6E12.8
9	RO(N)	6E12.8

The meaning of these program variables are as follows:

Variable	Description
TITLE	Title for identification of the problem.
NDBUG	Debug option NDBUG = 0 only results NDBUG = 1 includes intermediate computations
NETA	Length of input stepsize distribution.
NSP	Number of species.
NE	Number of elements.

Variable	Description
TOL	Convergence criteria for chemical equilibrium calculation. Recommended value is 0.001.
UINF	Freestream velocity (ft/sec).
DTIL	Transformed standoff distance.
RAD	Body radius (ft).
RINF	Freestream Density (lb/ft^3)
RZB	Density ratio across shock.
DELTA	Nondimensional standoff distance, δ.
ET(N)	Stepsize distribution, η.
YOND(N)	y/δ, distribution.
TT(N)	Temperature distribution(^{o}K).
PI(N)	Pressure distribution (atm).
W(N)	Velocity distribution (ft/sec).
RO(N)	Density distribution (ρ/ρ_s).

TABLE G-1

DESCRIPTION OF SLAM SUBPROGRAMS

Subprogram	Description	Additional Subprograms Required
MAIN	Driver Program	INPUT, STPZE, INIT, ELEMNT, CHEMEQ, DENSTY, DELTAY, MCD, EFLUX, DIJ, REDUCE, OUTPUT, COMP, PROFIL, PLOTIT, LRAD4.
INPUT STPZE	Data input.	none
INPUT STPZE	Increases number of steps such that the maximum change in temperature from one point to the next.	SPACE
SPACE	Transfers tabular data from one stepsize distribution to another.	INTRPL
INTRPL	Interpolation scheme.	none
INIT	Initialization routine--for further details see listing.	SG13

8

TABLE G-1 (continued)

Subprogram	Description	Additional Subprograms Required
SG13	Curve smoothing program.	none
ELEMNT	Solves elemental equations as described in Chapter V.	FGH, FGH_2, TRID
FGH, FGH_2	Three point difference formulas for first and second derivatives.	none
TRID	Solution to simultaneous linear equations with tri-diagonal coefficient matrix.	none
OUTPUT	Prints out elemental profiles.	none
CHEMEQ	Determines equilibrium compositions. See Appendix E.	ALTERY, THERMO, MATINV
ALTERY	Adjusts assumed compositions such that desired elemental ratios are obtained.	none
THERMO	Computes the free energy of the species.	none
MATINV	Matrix inversion and simultaneous solution of linear equation set.	none

TABLE G-1 (continued)

Subprogram	Description	Additional Subprograms Required
DENSTY	Computes density profiles from equilibrium compositions.	none
PROFIL	Prints out composition profile.	none
DELTAY	Determines derivatives of mole fractions for MCD.	FGH
MCD	Solves Stefan-Maxwell equations as described in Chapter V.	MATINV
EFLUX	Computes elemental mass fluxes from species mass fluxes.	none
DIJ	Estimates new effective elemental diffusion coefficient.	none
COMP	Converts from mole fraction to mass fraction or the reverse.	none
LRAD4	Punches data package for LRAD4 radiation program described in Reference 5.6.	none

```
C   * * * * * *    M A I N   * * * * * * * * * * * * * * * * * * * * * * *
C
C **    **      FLOW FIELD ANALYSIS WITH EQUILIBRIUM CHEMISTRY    **   **
C **    **      AND MULTICOMPONENT DIFFUSION.  11/20/70           **   **
C
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON /SCF/ NCHECK,ITER
      COMMON /FPSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA
      COMMON/SP1/SS,TOL,NDBUG
      ND=0
      ITER=0
      ITYPE=2
      CALL INPUT
      CALL STPZE(NETA)
      CALL INIT
      CALL ELEMNT
      CALL CHEMEQ(1,NETA)
      CALL DENSTY(ND)
      CALL ELEMNT
      CALL CHEMEQ(1,NETA)
      CALL DENSTY(ND)
C
  100 CONTINUE
      ITER=ITER + 1
      CALL ELEMNT
               IF(NDBUG.GT.0)CALL OUTPUT
               IF(ITER.EQ.1)NCHECK=99
               IF(NCHECK.LE.0.AND.ITER.GT.1)GOTO150
C
      CALL CHEMEQ(1,NETA)
               IF(NDBUG.GT.0)CALL PROFIL(ITYPE)
      CALL DELTAY(NETA,NSP)
      CALL MCD
      CALL EFLUX
      CALL DIJ
      GOTO100
```

```
C-----INCREMENTAL PROFILES HAVE CONVERGED FOR THE GIVEN DENSITY PROFILE..
C
 150  CONTINUE
C
C-----CHECK FOR DENSITY CONVERGENCE....
C
      CALL DENSTY(ND)
      IF(ND.GT.0)GOTO100
C
C-----IF DENSITY PROFILE HAS CONVERGED, PRINT OUT SOLUTION....
C
      CALL REDUCE(NETA)
      CALL OUTPUT
      CALL PROFIL(ITYPE)
      CALL COMP(ITYPE,NSP,NETA)
      CALL PROFIL(ITYPE)

      CALL LRAD4
 200  STOP
      END
```

```
C
      SUBROUTINE INPUT
      COMMON/PROP1/PI(200),PO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON/TITL/TITLE(20)
      COMMON/WT/SMW(20),AWT(5)
      COMMON/SP1/SS,TOL,NDBUG
      COMMON/ID/SP(20),EL(5)
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/EQ2/AA(20,5)
      COMMON/EQ3/IA(20,5)
      COMMON /BLOCK2/ SIG(20),EOK(20)
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA
      COMMON /VEL/ F(200),FC(200),ZZ(200),VV(200)
      COMMON /YL/ ET(200),YOND(200)
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      DOUBLE PRECISION NAME(7),PARM(8)
      DATA NAME/' SPECIES',' SMW ',' SIGMA ',' EOK ',' CWALL ',
     X ' CSHOCK ',' A(I,J) '/
      DATA PARM/' NETA ',' NSP ',' UINF ',' DTIL ',' RAD ',
     X          ' RINF ',' RZB ',' DELTA '/
C
C------READ IN TITLE CARD.....
C
      READ 99,TITLE
C
C------READ IN PARAMETER CARDS......
C
      READ 100,NDBUG,NETA,NSP,     NE
      READ 108,TOL,UINF,DTIL,RAD,RINF,RZB,DELTA
C
C------READ IN PROFILES....
C
      READ 102,(ET(I),I=1,NETA)
```

```
      READ 102,(YOND(I),I=1,NETA)                                      INPU 360
      READ 102,(TT(I),I=1,NETA)                                        INPU 370
      READ 102,(PI(I),I=1,NETA)                                        INPU 380
      READ 102,(VV(I),I=1,NETA)                                        INPU 390
      READ 102,(RO(I),I=1,NETA)                                        INPU 400
      DO5N=1,NETA                                                      INPU 410
 5    PRINT 206,ET(N),YOND(N),TT(N),PI(N),VV(N),RO(N)                  INPU 420
 206  FORMAT(2F8.4,4E12.4)                                             INPU 430
C                                                                      INPU 440
C-----READ IN SPECIES CARDS......                                      INPU 450
C                                                                      INPU 460
      DO10I=1,NSP                                                      INPU 470
      READ 101,SP(I),SMW(I),SIG(I),EOK(I),C(I,1),C(I,NETA)             INPU 480
     X,             (IA(I,J),J=1,NE)                                   INPU 490
      READ 103,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)        INPU 500
      READ 103,AI (I),BI (I),CI (I),DI (I),EI (I),FI (I),GI (I)        INPU 510
 10   CONTINUE                                                         INPU 520
C                                                                      INPU 530
C-----LIST INPUT DATA....                                              INPU 540
C                                                                      INPU 550
      PRINT99,TITLE                                                    INPU 560
      PRINT 205, PARM                                                  INPU 570
      PRINT 201,NETA,NSP,UINF,DTIL,RAD,RINF,RZB,DELTA                  INPU 580
      PRINT 205,NAME                                                   INPU 590
      DO30I=1,NSP                                                      INPU 600
 30   PRINT202,SP(I),SMW(I),SIG(I),EOK(I),C(I,1),C(I,NETA)             INPU 610
     X,             (IA(I,J),J=1,NE)                                   INPU 620
      PRINT200                                                         INPU 630
      DO40I=1,NSP                                                      INPU 640
      PRINT203,SP(I),AI (I),BI (I),CI (I),DI (I),EI (I),FI (I),GI (I)  INPU 650
 40   PRINT204,       AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I) INPU 660
      RETURN                                                           INPU 670
 99   FORMAT(20A4)                                                     INPU 680
 100  FORMAT(3I5,5X,5I1)                                               INPU 690
 101  FORMAT(1X,A4,5F10.5,5X,5I1)                                      INPU 700
 102  FORMAT(6E12.8)                                                   INPU 710
```

```
103   FORMAT(7E10.4)                                                          INPU 720
104   FORMAT(1X,A4,F10.5,I5)                                                  INPU 730
106   FORMAT(8E10.4)                                                          INPU 740
200   FORMAT(1H1,' SPECIES',35X,'THERMO-CONSTANTS A-G',29X,'RANGE')           INPU 750
201   FORMAT(2(4X,I2,4X),7E10.3)                                              INPU 760
202   FORMAT(2X,A4,2X,2F10.3,F10.1,2F10.5,5X,5I1)                             INPU 770
203   FORMAT(1X,A4,7E12.4,'  LOW RANGE')                                      INPU 780
204   FORMAT(      5X,7E12.4,'  HIGH RANGE')                                  INPU 790
205   FORMAT(/,8(1X,A8,1X))                                                   INPU 800
      END                                                                     INPU 810
```

```
C
      SUBROUTINE STPZE(NETA)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /VEL/ F(200),FC(200),ZZ(200),VV(200)
      COMMON /STPZ/ EN(200),NPT
      COMMON /YL/ ET(200),YOND(200)
      DIMENSION DUM(200)
C
C-----SET UP THE ETA DISTRIBUTION....
C
      EN(1)=0.0
      N=2
      NO=2
      TMAX=75.0
   10 DELT=ABS(TT(NO)-TT(NO-1))
      NSTEP=DELT/TMAX + 1.0
      I=0
      DELETA=(ET(NO)-ET(NO-1))/NSTEP
   15 EN(N)=EN(N-1) + DELETA
      I=I+1
      N=N+1
      IF(I.LT.NSTEP)GOTO15
      NO=NO+1
      IF(NO.LE.NETA)GOTO10
      N=N-1
      EN(N)=1.0
      NPT=N
      PRINT 99
   99 FORMAT(//,20X,' REVISED ETA DISTRIBUTION....',/)
      PRINT 101, (EN(I),I=1,NPT)
  101 FORMAT(10E12.4)
      CALL    SPACE(EN,NPT,ET,TT,NETA)
      CALL    SPACE(EN,NPT,ET,PI,NETA)
      CALL    SPACE(EN,NPT,ET,RO,NETA)
      CALL    SPACE(EN,NPT,ET,VV,NETA)
```

```
      CALL    SPACE(EN,NPT,ET,YOND,NETA)                                STPZ 360
C                                                                       STPZ 370
      DO45N=1,NETA                                                      STPZ 380
   45 DUM(N)=ET(N)                                                      STPZ 390
      DO46N=1,NPT                                                       STPZ 400
   46 ET(N)=EN(N)                                                       STPZ 410
      DO47N=1,NETA                                                      STPZ 420
   47 EN(N)=DUM(N)                                                      STPZ 430
      N=NETA                                                            STPZ 440
      NETA=NPT                                                          STPZ 450
      NPT=N                                                             STPZ 460
C                                                                       STPZ 470
      DO50I=1,NSP                                                       STPZ 480
   50 C(I,NETA)=C(I,NPT)                                                STPZ 490
C                                                                       STPZ 500
      DO60N=2,NETA                                                      STPZ 510
      IF(TT(N).GT.TT(N-1))GOTO60                                        STPZ 520
      TT(N)=TT(N-1)*.5 + TT(N+1)*.5                                     STPZ 530
   60 CONTINUE                                                          STPZ 540
      PRINT 100,NETA                                                    STPZ 550
  100 FORMAT(///' NETA=',I3)                                            STPZ 560
      RETURN                                                            STPZ 570
C                                                                       STPZ 580
C * * * * * * * * * * * * * * *                                         STPZ 590
      ENTRY REDUCE(NETA)                                                STPZ 600
C * * * * * * * * * * * * * * *                                         STPZ 610
C                                                                       STPZ 620
      CALL    SPACE(EN,NPT,ET,TT,NETA)                                  STPZ 630
      CALL    SPACE(EN,NPT,ET,PI,NETA)                                  STPZ 640
      CALL    SPACE(EN,NPT,ET,RO,NETA)                                  STPZ 650
      CALL    SPACE(EN,NPT,ET,VV,NETA)                                  STPZ 660
      CALL    SPACE(EN,NPT,ET,AMW,NETA)                                 STPZ 670
      CALL    SPACE(EN,NPT,ET,YOND,NETA)                                STPZ 680
C                                                                       STPZ 690
      DO75J=1,NE                                                        STPZ 700
      DO70N=1,NETA                                                      STPZ 710
```

```
  7   DUM(N)=CC(J,N)                                   STPZ 720
      CALL SPACE(EN,NPT,ET,DUM,NETA)                   STPZ 730
      DO75N=1,NPT                                      STPZ 740
 75   CC(J,N)=DUM(N)                                   STPZ 750
C                                                      STPZ 760
      DO80I=1,NSP                                      STPZ 770
      DO78N=1,NETA                                     STPZ 780
 78   DUM(N)=C(I,N)                                    STPZ 790
      CALL SPACE(EN,NPT,ET,DUM,NETA)                   STPZ 800
      DO80N=1,NPT                                      STPZ 810
 80   C(I,N)=DUM(N)                                    STPZ 820
C                                                      STPZ 830
      DO85N=1,NETA                                     STPZ 840
 85   DUM(N)=ET(N)                                     STPZ 850
      DO86N=1,NPT                                      STPZ 860
 86   ET(N)=EN(N)                                      STPZ 870
      DO87N=1,NETA                                     STPZ 880
 87   EN(N)=DUM(N)                                     STPZ 890
C                                                      STPZ 900
      N=NETA                                           STPZ 910
      NETA=NPT                                         STPZ 920
      NPT=N                                            STPZ 930
C                                                      STPZ 940
      RETURN                                           STPZ 950
C                                                      STPZ 960
      END                                              STPZ 970
```

```
      SUBROUTINE    SPACE(XNEW,NEW,X,Y,NOLD)
      DIMENSION XNEW(200),X(200),Y(200),DUM(200)
      DO10N=1,NEW
      XN=XNEW(N)
      CALL  INTRPL(XN,X,Y,NOLD,YN)
   10 DUM(N)=YN
      DO20N=1,NEW
   20 Y(N)=DUM(N)
      RETURN
      END
```

```
C
      SUBROUTINE INTRPL(VAR,X,F,IMAX,SOM)
C
C-----THIS PROGRAM PERFORMS LAGRANGIAN INTERPOLATION
C     WITH NON-EQUAL STEP SIZE BETWEEN POINTS
C     F=DEPENDENT VARIABLE
C     X=INDEPENDENT VARIABLE
C     VAR=VALUE OF X FOR WHICH CORRESPONDING VALUE OF
C     F IS DESIRED BY INTERPOLATION
C     IMAX=NUMBER OF POINTS IN ARRAY X OR F
C     SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE
C     NPTS=NUMBER OF POINTS USED FOR INTERPOLATION
C
      DIMENSION X(100),F(100),XN(300),FN(300)
      NPTS=7
  607 XUP=1.E30
      DO611 I=1,IMAX
      T=VAR-X(I)
      IF(T.GE.0.0)GO TO 609
  608 T=-T
  609 IF(T.GE.XUP)GO TO 611
  610 IP=I
      XUP=T
  611 CONTINUE
      IN=1
      NPP=NPTS+1
      DO618I=1,NPP
      FN(I)=F(IP)
      XN(I)=X(IP)
      IF(IN.GT.0)GO TO 613
  612 IQ=IP-I
      GO TO 615
  613 IQ=IP+I
      IF(IMAX.GE.IQ)GO TO 615
  614 IP=IP-1
      GO TO 618
```

```
615   IF(IQ.GT.0)GO TO 617
616   IP=IP+1
      GO TO 618
617   IP=IQ
      IN=-IN
618   CONTINUE
      SOM=0.0
      FACT=1.0
      DO620 J=1,NPTS
      SOM=SOM+FACT*FN(1)
      DO619 I=J,NPTS
      IQ=I-J+1
619   FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))
620   FACT=FACT*(VAR-XN(J))
      RETURN
      END
```

```
                                                                              INTR 520
C                                                                             INIT  10
      SUBROUTINE INIT                                                         INIT  20
      COMMON/NUMBER/NSE,NNS,NE,NC                                             INIT  30
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)INIT  40
      COMMON/WT/SMW(20),AWT(5)                                                INIT  50
      COMMON /WALL/ECWALL(5)                                                  INIT  60
      COMMON/EQ2/AA(20,5)                                                     INIT  70
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL                                INIT  80
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM, NETA          INIT  90
      COMMON/EQ3/IA(20,5)                                                     INIT 100
      COMMON /VEL/ F(200),FC(200),ZZ(200),VV(200)                             INIT 110
      COMMON /DIF/D(5,200)                                                    INIT 120
      COMMON /MCD1/JS(20,200),JE(5,200)                                       INIT 130
      COMMON /YL/ ET(200),YOND(200)                                           INIT 140
      DIMENSION DUM(200)                                                      INIT 150
      REAL JS, JE                                                             INIT 160
      TD=1.0                                                                  INIT 170
      RHOD=RINF/RZB                                                           INIT 180
      FACT=RHOD*.7604                                                         INIT 190
C                                                                             INIT 200
C-----FIRST NE SPECIES ARE ELEMENTS......                                     INIT 210
C                                                                             INIT 220
      DO5J=1,NE                                                               INIT 230
    5 AWT(J)=SMW(J)                                                           INIT 240
C                                                                             INIT 250
C-----SMOOTH AND NON-DIMENSIONALIZE VELOCITY PROFILE, GUESS INITIAL           INIT 260
C     AMW-PROFILE....                                                         INIT 270
C                                                                             INIT 280
      CALL SG13(ET,VV,DUM,NETA,IER)                                           INIT 290
      DO25N=1,NETA                                                            INIT 300
      VV(N)=DUM(N)/UINF                                                       INIT 310
      AMW(N)=RO(N)*FACT*TT(N)/PI(N)                                           INIT 320
   25 DUM(N)=TT(N)                                                            INIT 330
C                                                                             INIT 340
C-----SMOOTH TEMPERATURE PROFILE....                                          INIT 350
C
```

```
      CALL SGI3(ET,DUM,TT,NETA,IER)
C
C-----FLOAT AA(I,J) MATRIX....
C
      DO30I=1,NSP
      DO30J=1,NE
 30   AA(I,J)=IA(I,J)
C
C-----CONVERT WALL AND SHOCK COMPOSITIONS TO AN ELEMENTAL BASIS.....
C
      DO35N=1,NETA
      DO35J=1,5
 35   CC(J,N)=0.0
      DO24J=1,NE
      DO23I=1,NSP
      FAC=AA(I,J)*AWT(J)/SMW(I)
      CC(J,1)=CC(J,1) + FAC*C(I,1)
 23   CC(J,NETA)=CC(J,NETA) + FAC*C(I,NETA)
 24   ECWALL(J)=CC(J,1)
C
C-----ESTIMATE INITIAL ELEMENTAL DIFFUSION COEFFICIENTS....
C
      READ999,A
 999  FORMAT(E10.4)
      DO50J=1,NE
      DO50N=1,NETA
      JE(J,N)=0.0
 50   D(J,N)=A*(TT(N)**1.659)/(FI(N)*UINF*RAD)
      RETURN
      END
```

```
      SUBROUTINE SG13(X,Y,Z,NDIM,IER)
C
C
C        SUBROUTINE SG 13
C
C        PURPOSE
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN
C           VECTORS OF ARGUMENT VALUES AND CORRESPONDING FUNCTION
C           VALUES
C
C        USAGE
C           CALL SG13(X,Y,Z,NDIM,IER)
C
C        DESCRIPTION OF PARAMETERS
C           X      -   GIVEN VECTOR OF ARGUMENT VALUES (DIMENSION NDIM)
C           Y       -   GIVEN VECTOR OF FUNCTION VL
C           Y      - GIVEN VECTOR OF FUNCTION VALUES CORRESPONDING TO X
C                      (DIMENSION NDIM)
C           Z      -   RESULTING VECTOR OF SMOOTHED FUNCTION VALUES
C                      (DIMENSION NDIM)
C           NDIM    -  DIMENSION OF VECTORS X,Y,AND Z
C           IER     -  RESULTING ERROR PARAMETER
C                      IER = -1 - NDIM IS LESS THAN 3
C                      IER = 0 - NO ERROR
C        REMARKS
C           (1)  IF    IER=-1THERE HAS BEEN NO COMPUTATION.
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS X OR Y. IF
C                   X OR Y IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.
C        SUBROUTINES AND SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), EACH SMOOTHED
C           VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE LEAST-
C           SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 3 SUCCESSIVE
```

```
C             POINTS (X(I+K),Y(I+K),                                    SG13 370
C             POINTS (X(I+K),Y(I+K)) K =-1.0,1.(SEE HILDEBRAND,F.P.,    SG13 380
C             INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ SG13 390
C             TORONTO/LONDON, 1956, PP. 258-311.)                       SG13 400
C                                                                       SG13 410
C                                                                       SG13 420
      DIMENSION X(1),Y(1), Z(1)                                         SG13 430
C                                                                       SG13 440
C              TEST OF DIMENSION                                        SG13 450
      IF(NDIM-3)7,1,1                                                   SG13 460
C                                                                       SG13 470
C            START LOOP                                                 SG13 480
    1 DO 6 I=3,NDIM                                                     SG13 490
         XM=.3333333*(X(I-2)+X(I-1)+X(I))                               SG13 500
         YM=.3333333*(Y(I-2)+Y(I-1)+Y(I))                               SG13 510
         T1=X(I-2)-XM                                                   SG13 520
         T2=X(I-1)-XM                                                   SG13 530
         T3=X(I)-XM                                                     SG13 540
         XM=T1*T1+T2*T2+T3*T3                                           SG13 550
      IF(XM)3,3,2                                                       SG13 560
    2 XM=(T1*(Y(I-2)-YM)+T2*(Y(I-1)-YM)+T3*(Y(I)-YM))/XM                SG13 570
C                                                                       SG13 580
C             CHECK FIRST POINT                                         SG13 590
    3 IF(I-3)4,4,5                                                      SG13 600
    4 H=XM*T1+YM                                                        SG13 610
    5 Z(I-2)=H                                                          SG13 620
    6 H=XM*T2+YM                                                        SG13 630
C             END OF LOOP                                               SG13 640
C                                                                       SG13 650
C             UPDATE LAST TWO COMPONENTS                                SG13 660
      Z(NDIM-1)=H                                                       SG13 670
         IER=0                                                          SG13 680
         IER=1                                                          SG13 690
      Z(NDIM)=XM*T3+YM                                                  SG13 700
      RETURN                                                            SG13 710
C                                                                       SG13 720
```

```
C              ERROR EXIT IN CASE NDIM IS LESS THAN 3                    SG13 730
    7  IER=-1                                                            SG13 740
       RETURN                                                            SG13 750
       END                                                               SG13 760
```

```
BLOCK DATA                                                    DATA 10
COMMON/ID/SP(20),BL(5)                                        DATA 20
DATA SP/20*'     '/                                           DATA 30
END                                                           DATA 40
```

```
C                                                                       DATA  50
      SUBROUTINE ELEMNT                                                 ELEM  10
      COMMON /WALL/ECWALL(5)                                            ELEM  20
      COMMON/WT/SMW(20),AWT(5)                                          ELEM  30
      COMMON/NUMBER/NS,NNS,NE,NCC                                       ELEM  40
      COMMON /MCD1/JS(20,200),JE(5,200)                                 ELEM  50
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)ELEM  60
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM, NETA   ELEM  70
      COMMON /VECTOR/SUB(200),DIAG(200),SUP(200),B(200)                 ELEM  80
      COMMON /SCE/ NCHECK,ITER                                          ELEM  90
      COMMON/SP1/SS,TOL,NDBUG                                           ELEM 100
      COMMON /DIF/D(5,200)                                              ELEM 110
      COMMON /YL/ ET(200),YOND(200)                                     ELEM 120
      COMMON /VFL/FF(200),FC(200),ZZ(200),VV(200)                       ELEM 130
      COMMON /DEL/ DELTA,DTIL,DTILS                                     ELEM 140
      COMMON/FUNCTN/DROV(200),X(200)                                    ELEM 150
      DIMENSION TEF(5,200)                                              ELEM 160
      DIMENSION XM(5)                                                   ELEM 170
      REAL JS, JE                                                       ELEM 180
      M=1                                                               ELEM 190
      NCHECK=0                                                          ELEM 200
      NM1=NETA-1                                                        ELEM 210
      DO15J=1,NE                                                        ELEM 220
 15   XM(J)=RO(1)*VV(1)*ECWALL(J)                                       ELEM 230
C                                                                       ELEM 240
C-----SOLVE ELEMENTAL SPECIES EQUATIONS IN A GLOBALLY IMPLICIT MATTER...ELEM 250
C                                                                       ELEM 260
 150  DO180J=1,NE                                                       ELEM 270
      DIAG(1)=DTIL*VV(1)*ET(2)/(RO(1)*D(J,1)) + 1.0                     ELEM 280
      SUP(1)=-1.0                                                       ELEM 290
      B(1)=XM(J)*DTIL*ET(2)/(RO(1)*RO(1)*D(J,1))                        ELEM 300
C                                                                       ELEM 310
 154  DO155K=2,NETA                                                     ELEM 320
      N=M-1+K                                                           ELEM 330
      CALL FGH(N,F1,G1,H1)                                              ELEM 340
      CALL FGH2(N,F2,G2,H2)                                             ELEM 350
```

```
      DLNRO=F1*RO(N+1)/RO(N) + G1 + H1*RO(N-1)/RO(N)                    ELEM 360
      PETA=-DTIL*VV(N)/(RO(N)*D(J,N)) + 2.*DLNRO                        ELEM 370
      SUB(K-1)= PETA*H1 + H2                                            ELEM 380
      DIAG(K)= PETA*G1 + G2                                             ELEM 390
      SUP(K)= PETA*F1 + F2                                              ELEM 400
      B(K)=0.0                                                          ELEM 410
      IF(N.GE.(NETA-1))GOTO160                                          ELEM 420
155   CONTINUE                                                          ELEM 430
160   B(K)=-SUP(K)*CC(J,NETA)                                           ELEM 440
      CALL TRID(K)                                                      ELEM 450
      DO170L=1,K                                                        ELEM 460
      ERR=ABS(B(L)-CC(J,M-1+L))                                         ELEM 470
      IF(ERR.GT..025)NCHECK=NCHECK+1                                    ELEM 480
170   CC(J,M-1+L)=B(L)                                                  ELEM 490
180   CONTINUE                                                          ELEM 500
      IF(NE.LT.5)GOTO1100                                               ELEM 510
1000  CC(5,N)=(CC(1,N)/AWT(1) + CC(3,N)/AWT(3) + CC(4,N)/AWT(4))*AWT(5) ELEM 520
1100  CONTINUE                                                          ELEM 530
      RETURN                                                            ELEM 540
      END                                                               ELEM 550
```

```
C                                                                               ELEM 560
      SUBROUTINE FGH(N,F,G,H)                                                   FGH(  10
C  **     **    FIRST DERIVATIVE    **     **     **                            FGH(  20
C------EVALUATES COEFFICIENTS FOR THREE POINT DIFFERENCE APPROXIMATION          FGH(  30
C       OF DAVIS (AIAA JR. VOL. 8, NO. 5, MAY 1970).                            FGH(  40
      COMMON /YL/ ET(200),YOND(200)                                             FGH(  50
      DN=ET (N+1)-ET (N)                                                        FGH(  60
      DNM1=ET (N)-ET (N-1)                                                      FGH(  70
      DEL=DN+DNM1                                                               FGH(  80
      D1=DN*DEL                                                                 FGH(  90
      D2=DN*DNM1                                                                FGH( 100
      D3=DNM1*DEL                                                               FGH( 110
      F=DNM1/D1                                                                 FGH( 120
      G=(DN-DNM1)/D2                                                            FGH( 130
      H=-DN/D3                                                                  FGH( 140
      RETURN                                                                    FGH( 150
      END                                                                       FGH( 160
```

```
      SUBROUTINE FGH2(N,F,G,H)
C   **     **     SECOND DERIVATIVE    **     **     **
C------EVALUATES COEFFICIENTS FOR THREE POINT DIFFERENCE APPROXIMATION
C       OF DAVIS (AIAA JR. VOL. 8, NO. 5, MAY 1970).
      COMMON /YL/ ET(200),YOND(200)
      DN=ET (N+1)-ET (N)
      DNM1=ET (N)-ET (N-1)
      F=2./(DN*(DN+DNM1))
      G=-2./(DN*DNM1)
      H=2./(DNM1*(DN+DNM1))
      RETURN
      END
```

```
C
      SUBROUTINE TRID (M)
C**** TRID --TRIDIAGONAL EQUATION SOLVER  OBTAINED FROM CONTE P-184 ***
C      SUBROUTINE SOLVES AX = B FOR THE VECTOR X (WHERE A IS TRIDIAGONAL
C      M = ORDER OF SYSTEM
C      SUP = SUPER DIAGONAL OF A
C      SUB = SUB DIAGONAL OF A
C      DIAG = MAIN DIAGONAL OF A
C      B = CONSTANT VECTOR
C      SUP AND DIAG ARE DESTROYED
C      SOLUTION VECTOR IS RETURNED IN B
C
      COMMON /VECTOR/SUB(200),DIAG(200),SUP(200),B(200)
C
      N = M
      NN = N -1
      SUP(1) = SUP(1)/DIAG(1)
      B(1) = B(1)/DIAG(1)
      DO 10 I=2,N
      II = I -1
C------DECOMPOSE A TO FORM A = LU WHERE L IS LOWER TRIANGULAR,
C      AND U IS UPPER TRIANGULAR ---------
      DIAG(I) = DIAG(I) - SUP(II)*SUB(II)
      IF(I .EQ. N) GO TO 10
      SUP(I) = SUP(I) / DIAG(I)
C------COMPUTE Z WHERE LZ = B
   10 B(I) = (B(I) - SUB(II) *B(II))/ DIAG(I)
C------COMPUTE X BY BACK SUBSTITUTION WHERE UX = Z
      DO 20 K =1,NN
      I = N - K
   20 B(I) = B(I) -SUP(I) *B(I+1)
      RETURN
      END
```

```
C
      SUBROUTINE OUTPUT
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NT
      COMMON /VEL/ F(200),FC(200),ZZ(200),VV(200)
      COMMON /YL/ ET(200),YOND(200)
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /SCE/ NCHECK,ITER
      DOUBLE PRECISION NAME(9)
      DATA NAME/' CARBON ','HYDROGEN','NITROGEN',' OXYGEN ','ELECTRON',
     1          '  T(CK) ','VELOCITY','  Y/D   ',' DENSITY'/
      IF(NCHECK.GT.0)PRINT 104,ITER
      IF(NCHECK.LE.0)PRINT 102,ITER
      PRINT 103
      PRINT 100,NAME
      DO5N=1,NT
    5 PRINT 101,ET(N),(CC(I,N),I=1,5),TT(N),VV(N),YOND(N),RO(N)
      RETURN
  100 FORMAT(     5X,'ETA',3X,9(2X,A8,2X))
  101 FORMAT(F10.4,1X,9E12.4)
  102 FORMAT( 1H1,1X,'MULTICOMPONENT SOLUTION CONVERGED IN ',I2,' ITERATI
     XONS'/)
  103 FORMAT( 15X,14('*'),'ELEMENTAL MASS FRACTIONS',15('*'))
  104 FORMAT(///,' ITERATION NUMBER ',I2)
      END
```

```
C
      SUBROUTINE CHEMEQ( NI,NF)
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C                                                                     *
C     THIS SUBPROGRAM IS A REVISION OF A PROGRAM ORIGINALLY REPORTED  *
C     IN J.CHEM.PHYS.,VOL.28,NO.5,1958.  THE PROGRAM COMPUTES FOR A   *
C     PRESSURE ARRAY,PP(N),TEMPERATURE ARRAY,TT(N), AND AN ARRAY      *
C     OF ELEMENTAL MASS FRACTIONS-CC(I,N), THE EQUILIBRIUM SPECIES    *
C     MASS FRACTIONS AT EACH POINT-N REPRESENTED BY THE GIVEN ARRAYS. *
C     THE EQUILIBRIUM COMPOSITIONS ARE STORED IN THE MATRIX CE(I,N).  *
C                                                                     *
C                                 DONALD D. ESCH                      *
C                                 LOUISIANA STATE UNIVERSITY          *
C                                                                     *
C                                 AUGUST 7, 1970                      *
C                                                                     *
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C     IN = INITIAL POINT FOR EQUILIBRIUM CALCULATIONS.                *
C     NF = FINAL POINT.                                               *
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
      COMMON/SP1/SS,TOL,NDBUG
      COMMON/PROP1/PP(200),RD(200),TT(200),AMW(200),CE(20,200),CC(5,200)
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/EQ2/AA(20,5)
      COMMON/THERM1/C(20),FORT(20)
      COMMON/ID/SP(20),EL(5)
      COMMON/NUMBER/NS ,NNS,MM,NC
      COMMON/WT/XMW(20),AWT(5)
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HIOTAL
      DIMENSION P(20,20),B(20,1),YINT(20),FY(20),PI(7),FSUM(20),YSUM(20)
     1 ,X(20),DELT(20),XLAM(20)
      DIMENSION E(5),BB(5),Y(20)
C
      MA=1
C
```

```
C-----INITIAL GUESS FOR EQUILIBRIUM CALCULATIONS....
C
      DO10I=1,NS
      IF(CE(I,NI).LE.0.0)CE(I,NI)=1.0E-10
 10   Y(I) = CE(I,NI)*AMW(NI)/XMW(I)
C
C-----COMPUTE THE SIZE OF THE MATRIX
C
      NA=MM+1
C
C     NS=NUMBER OF SPECIES....
C
C     CRIT=CRITERIA FOR CONVERGENCE.
C
      CRIT=1.E-4
      CRIT=.001
      XBETA=CRIT
      BETA=0.
      LL=NS+1
      TOLD=0.0
C
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
      DO500N=NI,NF
      T = TT(N)*TD
      P=PP(N)
      NT=1
      BETOLD=0.0
      SUM=0.0
      DO15I=1,MM
 15   SUM=SUM + CC(I,N)
      DO20 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(F,Y,TOLD)
C
      IF(ABS(T-TOLD).LE.50.)GOTO80C
C
      DO22I=1,NS
      IF(Y(I).LT.1.0E-8)Y(I)=1.0E-8
 22   CONTINUE
C
      DO25 J=1,MM
      BB(J)=0.C
      DO 25  I=1,NS
 25   BB(J)=BB(J)+AA(I,J)*Y(I)
C
      CALL THERMO(T,P)
C
C-----THERMO SUBROUTINE CALCULATES THE FREE ENRGY FUNCION.THE HEAT OF
C     FORMATION OF EVERY CHEMICAL SPECIE AT ANY TEMPERATURE T....
C
C
C-----SET-UP THE R-MATRIX AND THE B-VECTOR....
C
 40   YBAR=0.
      DO50I=1,NS
   50 YBAR=YBAR+Y(I)
C
C     YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES
C
C
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES
C
      DO60I=1,NS
      FAC=Y(I)/YBAR
      IF(FAC.LT.1.E-73)FAC=1.E-73
 60   FY(I)=Y(I)*(C(I)+ALOG(FAC)) .
C
```

```
C-----PROCEED TO CONSTRUCT THE R MATRIX                          CHEM1080
C                                                                CHEM1090
C-----INITIALIZE TO ZERO....                                     CHEM1100
C                                                                CHEM1110
      DO75J=1,NA                                                 CHEM1120
      DO75K=1,NA                                                 CHEM1130
   75 R(J,K)=0.0                                                 CHEM1140
C                                                                CHEM1150
      DO90J=1,MM                                                 CHEM1160
      DO90K=J,MM                                                 CHEM1170
      SUM=0.                                                     CHEM1180
      DO80I=1,NS                                                 CHEM1190
   80 SUM=SUM+AA(I,J)*AA(I,K)*Y(I)                               CHEM1200
      R(J,K)=SUM                                                 CHEM1210
   90 R(K,J)=SUM                                                 CHEM1220
C                                                                CHEM1230
      DO 103 K=1,MM                                              CHEM1240
      SUM=0.                                                     CHEM1250
      DO 101 I=1,NS                                              CHEM1260
  101 SUM=SUM+AA(I,K)*Y(I)                                       CHEM1270
      R(K,NA)=SUM                                                CHEM1280
      R(NA,K)=SUM                                                CHEM1290
  103 CONTINUE                                                   CHEM1300
C                                                                CHEM1310
C ----PROCEED TO CALCULATE THE VECTOR B.                         CHEM1320
C                                                                CHEM1330
      DO140J=1,MM                                                CHEM1340
      SUM=0.                                                     CHEM1350
      DO130I=1,NS                                                CHEM1360
  130 SUM=SUM+AA(I,J)*FY(I)                                      CHEM1370
  140 B(J,1)=SUM+BB(J)                                           CHEM1380
C                                                                CHEM1390
      SUM=0.                                                     CHEM1400
      DO150I=1,NS                                                CHEM1410
  150 SUM=SUM+FY(I)                                              CHEM1420
      B(NA,1)=SUM                                                CHEM1430
```

```
C                                                                       CHEM1440
C-----MATRIX INVERSION IS CALLED TO PROVIDE THE SOLUTION FOR             CHEM1450
C     THE LINEARIZED EQUATIONS. THE SOLUTION OF THE EQUATIONS           CHEM1460
C     GIVES THE LAGRANGIAN MULTIPLIERS NEEDED TO COMPUTE THE MOLES      CHEM1470
C     OF EACH GAS SPECIES.                                              CHEM1480
C                                                                       CHEM1490
      CALL MATINV(R,NA,B,MA,NMAX)                                       CHEM1500
 156  CONTINUE                                                          CHEM1510
C                                                                       CHEM1520
      DO160I=1,NA                                                       CHEM1530
C                                                                       CHEM1540
C     PI(I)=LAGRANGINA MULTIPLIERS                                      CHEM1550
C                                                                       CHEM1560
  160 PI(I)=B(I,1)                                                      CHEM1570
      U=PI(NA)                                                          CHEM1580
      XBAR=U*YBAR                                                       CHEM1590
C                                                                       CHEM1600
C-----COMPUTE THE MOLES OF EACH SPECIE....                              CHEM1610
C                                                                       CHEM1620
C                                                                       CHEM1630
      DO170I=1,NS                                                       CHEM1640
 170  FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR                                   CHEM1650
      DO200I=1,NS                                                       CHEM1660
      PSUM=0.                                                           CHEM1670
      DO180J=1,MM                                                       CHEM1680
 180  PSUM=PSUM+PI(J)*AA(I,J)                                           CHEM1690
      YSUM(I)=PSUM*Y(I)                                                 CHEM1700
 200  X(I)=FSUM(I)+YSUM(I)                                              CHEM1710
C                                                                       CHEM1720
C-----CHECK IF CONVERGENCE CRITERIA HAS BEEN MET. IF SO, GO TO 800      CHEM1730
C                                                                       CHEM1740
      BETA=0.0                                                          CHEM1750
      DO215I=1,NS                                                       CHEM1760
      DELT(I)=X(I)-Y(I)                                                 CHEM1770
 215  BETA=BETA+ABS(DELT(I))                                            CHEM1780
      IF(BETA.GT.BETOLD)GOTO216                                         CHEM1790
```

```
      IF(BETA.LT.XBETA)GOTO800                                    CHEM1800
 200  CONTINUE                                                    CHEM1810
C                                                                 CHEM1820
C-----COMPUTE THE CONVERGENCE PARAMENTER XLAMBD                   CHEM1830
C                                                                 CHEM1840
      XLAMBD=1.                                                   CHEM1850
      DO210 I=1,NS                                                CHEM1860
      IF(ABS(DELT(I)).LT.1.0E-20)DELT(I)=0.0                      CHEM1870
      IF(DELT(I).GE.0.)GOTO210                                    CHEM1880
      IF(X(I).GT.0.)GOTO210                                       CHEM1890
      XLAM(I)=-Y(I)/DELT(I)                                       CHEM1900
      XLAMBD=AMIN1(XLAMBD,XLAM(I))                                CHEM1910
      XLAMBD=.99*XLAMBD                                           CHEM1920
 210  CONTINUE                                                    CHEM1930
      XLAM1=XLAMBD                                                CHEM1940
      IF(XLAM1.EQ.0.)XLAM1=1.0E-5                                 CHEM1950
      DEBAR=0.                                                    CHEM1960
      DO220I=1,NS                                                 CHEM1970
 220  DEBAR=DEBAR+DELT(I)                                         CHEM1980
C                                                                 CHEM1990
C-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.               CHEM2000
C     APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE  CHEM2010
C     NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE  CHEM2020
C     VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF  CHEM2030
C     Y(I) AS WAS USED IN THE PREVIOUS ITERATION                  CHEM2040
C                                                                 CHEM2050
C                                                                 CHEM2060
C-----DETERMINE THE FREE ENERGY GRADIENT.  IF POSITIVE REDUCE XLAMBDA  CHEM2070
C     DFDL=FREE ENERGY GRADIENT                                   CHEM2080
C                                                                 CHEM2090
 230  DFDL=0.                                                     CHEM2100
      DO280I=1,NS                                                 CHEM2110
      FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)               CHEM2120
C     IF(FAC.GT.0.)GOTO260                                        CHEM2130
C     XLAMBD=.9*XLAMBD                                            CHEM2140
C     GOTO230                                                     CHEM2150
```

```
 260  DERP=(DELT(I)*YBAR-DEBAR*Y(I))/(YBAR+XLAMBD*DEBAR)                   CHEM2160
      IF(FAC.LT.1.E-73)FAC=1.E-73                                          CHEM2170
 280  DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC)) + DERP                            CHEM2180
      IF(DFDL.LT.0.000)GOTO300                                             CHEM2190
      XLAMBD=.8*XLAMBD                                                     CHEM2200
      IF(XLAMBD.GT.1.0E-08)GOTO230                                         CHEM2210
C                                                                          CHEM2220
C-----THE VALUE OF XLAMBD THAT ASSURES CONVERGENCE HAS BEEN FOUND         CHEM2230
C                                                                          CHEM2240
 300  DO350I=1,NS                                                          CHEM2250
      IF(XLAMBD.GT.1.E-6)GOTO330                                           CHEM2260
      IF(DFDL.LT.0.)GOTO330                                                CHEM2270
      IF(XLAM1.LT.1.E-6)XLAM1=1.E-6                                        CHEM2280
C                                                                          CHEM2290
C-----CALCUALTE THE NEW COMPOSITION FOR THE NEXT ITERATION                CHEM2300
C                                                                          CHEM2310
      Y(I)=Y(I)+XLAM1*DELT(I)*.1                                           CHEM2320
      GOTO340                                                              CHEM2330
 330  Y(I)=Y(I)+XLAMBD*DELT(I)                                             CHEM2340
 340  IF(Y(I).LT.0.)Y(I)=1.E-73                                            CHEM2350
 350  CONTINUE                                                             CHEM2360
C                                                                          CHEM2370
 532  NT=NT+1                                                              CHEM2380
      BETOLD=BETA                                                          CHEM2390
      TOLD=T                                                               CHEM2400
C                                                                          CHEM2410
C-----IF THE NUMBER OF ITERATIONS EXCEED 900 STOP COMPUTATIONS            CHEM2420
C                                                                          CHEM2430
      IF(NT.GT.900)GOTO6000                                                CHEM2440
      GOTO40                                                               CHEM2450
 800  CONTINUE                                                             CHEM2460
C                                                                          CHEM2470
C-----CONVERT Y(I) TO MOLE FRACTIONS.....                                  CHEM2480
C                                                                          CHEM2490
C      THESE VALUES IN THE CF-MATRIX.  AMW(N) IS THE AVERAGE MOLECULAR     CHEM2500
C      CONVERT EQUILIBRIUM MOLE FRACTIONS TO MASS FRACTIONS AND STORE      CHEM2510
```

```
C     WEIGHT AT THE POINT, N.                                           CHEM2520
C                                                                       CHEM2530
      SUMY=0.0                                                          CHEM2540
      DO900I=1,NS                                                       CHEM2550
  900 SUMY=SUMY+Y(I)                                                    CHEM2560
      AMW(N) = 0.0                                                      CHEM2570
      DO1000I=1,NS                                                      CHEM2580
      Y(I)=Y(I)/SUMY                                                    CHEM2590
 1000 AMW(N) = AMW(N) + Y(I)*XMW(I)                                     CHEM2600
      DO1005I=1,NS                                                      CHEM2610
 1005 CE(I,N) = Y(I)                                                    CHEM2620
C1005 CE(I,N) = Y(I)*XMW(I)/AMW(N)                                      CHEM2630
C                                                                       CHEM2640
C     OPTIONAL OUTPUT OF POSITION , TEMPERATURE AND EQUILIBRIUM         CHEM2650
C     COMPOSITIONS.                                                     CHEM2660
C                                                                       CHEM2670
      IF(NDBUG.LT.3)GOTO3300                                            CHEM2680
      PRINT 2000,P,TT(N),NT                                             CHEM2690
 2000 FORMAT(//,'  P = ',F5.3,' T(OK) = ',F6.0,5X,'NUMBER OF ITERATIONS CHEM2700
     X='I3,//,11X,'Y(I)',12X,'C(I,N)',/)                                CHEM2710
      PRINT 2005,(SP(I),Y(I),CE(I,N),I=1,NS)                            CHEM2720
 2005 FORMAT(1X,A4,2E18.8)                                              CHEM2730
C                                                                       CHEM2740
 3300 XBETA=CRIT                                                        CHEM2750
 5000 CONTINUE                                                          CHEM2760
      RETURN                                                            CHEM2770
 6000 PRINT6001                                                         CHEM2780
 6001 FORMAT( ' NUMBER OF ITERATIONS EXCEEDED 900, PROGRAM TERMINATING')CHEM2790
      RETURN                                                            CHEM2800
      END                                                               CHEM2810
```

```
C
      SUBROUTINE ALTERY(F,Y,TOLD)
      COMMON/WT/SMW(20),AWT(5)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON/EQ2/AA(20,5)
      COMMON /SP1/SS,TOL,NDBUG
      DIMENSION E(5),Y(20),B(5),EOLD(5)
      DATA EOLD/5*0.0/
C
C-----CHECK TO SEE IF ELEMENTAL COMPOSITION HAS CHANGED SIGNIFICANTLY.
C     IF NOT, THEN RETURN......
C
      CHANGE=0.0
      DO5J=1,NE
      CHANGE=CHANGE+ABS(EOLD(J)-E(J))
 5    EOLD(J)=E(J)
      IF(CHANGE.LT.1.0E-4)RETURN
C
C-----ASSUME ALL SPECIES HAVE THE SAME COMPOSITION......
C
C
C-----COMPUTE GRAM-ATOMS OF EACH ELEMENT FROM KNOWN ELEMENTAL CPMPOS
C     DISTRIBUTION AND THE MAXIMUM POSSIBLE MOLECULAR WEIGHT......
C
      DO20J=1,NE
      IF(E(J).GT.1.0E-8)GOTO20
      DO15I=1,NSP
      IF(AA(I,J).LE.0.0)GOTO15
      Y(I)=1.0E-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
C     FIRST GUESS.  ADJUST THE COMPOSITION OF EACH ELEMENT-SPECIE AS
C     REQUIRED......
C
```

```
      DO30J=1,NE                                                      ALTE 360
      B(J)=0.0                                                        ALTE 370
      DO30I=1,NSP                                                     ALTE 380
30    B(J)=B(J)+AA(I,J)*Y(I)                                          ALTE 390
      DO40J=1,NE                                                      ALTE 400
40    Y(J)=Y(J)            + (E(J)-B(J))                              ALTE 410
      TOLD=0.0                                                        ALTE 420
      RETURN                                                          ALTE 430
      END                                                             ALTE 440
```

```
C
      SUBROUTINE THERMC(T,P)
C
C
C-----SUBROUTINE THERMC CALCULATES THE FREE ENERGY FUNCTION FOR EACH
C     CHEMICAL SPECIE.
C
C
      COMMON/NUMBER/NQ ,NNS,NE,NC
      COMMON/EQ1/AI(20), BI(20), CI(20), DI(20), EI(20), FI(20), GI(20),
     X          AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20)
      COMMON/THERM1/C(20),FORT(20)
C
C     T=TEMPERATURE IN OK
C
      T1=T
      T2=T1*T
      T3=T2*T
      T4=T3*T
      T5=T4*T
C
C
C-----CALCUALTE THE FREE ENERGY FUNCTION FORT(I)
C
C     FORT(I)=FREE ENERGY FUNCTION
C
      DO 41 I=1,NQ
      IF(T.GT.7000.   )GOTO6205
      FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.
     1        -EI(I)*T4/20.+FI(I)/T-GI(I)
      C(I)=FORT(I)+ALOG(P)
      IF(T.LT.7000)GOTO41
      FLOW=FORT(I)
      CLOW=C(I)
 6205 FORT(I)=AII(I)*(1.-ALOG(T))-BII(I)*T/2.-CII(I)*T2/6.-DII(I)*T3/12.
     1        -EII(I)*T4/20.+FII(I)/T-GII(I)
```

```
      C(I)=FORT(I)+ALOG(P)                                              THER 360
      IF(T.GT.7000)GOTO41                                               THER 370
      FAC=(T-5000.)/2000.                                               THER 380
      FORT(I)=FORT(I)*FAC + FLOW*(1.0-FAC)                              THER 390
      C(I)=C(I)*FAC + CLOW*(1.0-FAC)                                    THER 400
   41 CONTINUE                                                          THER 410
      RETURN                                                            THER 420
      END                                                               THER 430
```

```
C                                                                         CHEM2820
      SUBROUTINE MATINV(A,N,B,M,NMAX)
C
C
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
      DIMENSION A(20,20),B(20,1),IPIVOT(20),INDEX(20,2)
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)
C
C     INITIALIZATION
C
    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)=0
   30 DO 550 I=1,N
C
C     SEARCH FOR PIVOT ELEMENT
C
   40 AMAX=0.0
   45 DO 105 J=1,N
   50 IF (IPIVOT(J)-1)60,105,60
   60 DO 100 K=1,N
   70 IF (IPIVOT(K)-1)80,100,740
   80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100
   85 IROW=J
   90 ICOLUM=K
   95 AMAX=A(J,K)
  100 CONTINUE
  105 CONTINUE
      IF (AMAX)110,106,110
  106 DETERM=0.0
      ISCALE=0
      GO TO 740
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
```

```
C
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
  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
C     SCALE THE DETERMINANT
C
 1000 PIVOTI=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(PIVOTI)-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(ICOLUM,ICOLUM)=1.0
  340 DO 350 L=1,N
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT
  355 IF(M) 380,380,360
  360 DO 370 L=1,M
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT
C
C     REDUCE NON-PIVOT ROWS
C
  380 DO 550 L1=1,N
  390 IF(L1-ICOLUM)400,550,400
  400 T=A(L1,ICOLUM)
  420 A(L1,ICOLUM)=0.0
  430 DO 450 L=1,N
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
  455 IF(M) 550,550,460
  460 DO 500 L=1,M
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
  550 CONTINUE
C
C     INTERCHANGE COLUMNS
```

```
  600 DO 710 I=1,N                                              MATI1080
C                                                               MATI1090
  610 L=N+1-I                                                   MATI1100
  620 IF(INDEX(L,1)-INDEX(L,2))630,710,630                      MATI1110
  630 JROW=INDEX(L,1)                                           MATI1120
  640 JCOLUM=INDEX(L,2)                                         MATI1130
  650 DO 705 K=1,N                                              MATI1140
  660 SWAP=A(K,JROW)                                            MATI1150
  670 A(K,JROW)=A(K,JCOLUM)                                     MATI1160
  700 A(K,JCOLUM)=SWAP                                          MATI1170
  705 CONTINUE                                                  MATI1180
  710 CONTINUE                                                  MATI1190
  740 RETURN                                                    MATI1200
      END                                                       MATI1210
```

```
C
      SUBROUTINE DENSTY(ND)
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      COMMON /FRSTPM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA
      COMMON /YL/ ET(200),YOND(200)
      DIMENSION RS(200)
      DEN=RZB*.7604/RINF
      ND=0
      DO10N=1,NETA
      RNEW=DEN*AMW(N)*PI(N)/TT(N)
      ERR=(RNEW-RO(N))/RO(N)
      IF(ABS(ERR).GT..05)ND=ND+1
   10 RO(N)=RNEW*.7 + RO(N)*.3
      RETURN
      END
```

```
C
      SUBROUTINE PROFIL(ITYPE)
      COMMON /YL/ ET(200),YOND(200)
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON /VEL/ F(200),FC(200),ZZ(200),VV(200)
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON/ID/SP(20),EL(5)
      DIMENSION TYPE(2)
      DATA TYPE/'MASS','MOLE'/
      PRINT 200
      PRINT 201,TYPE(ITYPE),(SP(I),I=1,10)
      DO10N=1,NETA
      NCP=10
      IF(NSP.LT.10)NCP=NSP
   10 PRINT 202, ET(N),(C(I,N),I=1,NCP)
      IF(NSP.LE.10)GOTO30
      PRINT 200
      PRINT 201,TYPE(ITYPE),(SP(I),I=11,NSP)
      DO20N=1,NETA
   20 PRINT 202, ET(N),(C(I,N),I=11,NSP)
   30 RETURN
  200 FORMAT(1H1)
  201 FORMAT( ' EQUILIBRIUM ',A4,' FRACTIONS'/'  ETA ',2X,10(5X,A4,3X))
  202 FORMAT(1X,F6.4,10E12.4)
      END
```

```
C
      SUBROUTINE DELTAY(NETA,NSP)
      COMMON /DELY/ DY(20,200)
      COMMON /YL/ ET(200),YOND(200)
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      NM1=NETA-1
      DO10N=2,NM1
      CALL FGH(N,F,G,H)
      DO10I=1,NSP
   10 DY(I,N)=F*C(I,N+1) + G*C(I,N) + H*C(I,N-1)
      DO20I=1,NSP
      DY(I,NETA)=DY(I,NM1)
   20 DY(I,1)=DY(I,2)
      RETURN
      END
```

```
C
      SUBROUTINE MCD
C------SOLVES FOR FLUXES FROM STEFAN-MAXWELL EQUATION AND SPECIFIED
C       COMPOSITION PROFILES....
      COMMON /DELY/ DY(20,200)
      COMMON /MCD1/JS(20,200),JE(5,200)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON/SP1/SS,TCL,NDBUG
      COMMON/WT/SMW(20),AWT(5)
      COMMON/ID/SP(20),EL(5)
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA
      COMMON /BLOCK2/ SIG(20),EOK(20)
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),Y (20,200),CC(5,200)
      COMMON /YL/ ET(200),YOND(200)
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /RH/ DUD,DPHI,TD,RZB,PD,HD,HTOTAL
      REAL JS,JE,LAMBDA,M12
      DIMENSION A(20,20),B(20,1),D(20,20),L(20)
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C-----INITIALIZATION......
C
      NM1=NETA-1
      DO2I=1,NSP
      Y(I,NETA+1)=Y(I,NETA)
      JS(I,NETA)=0.0
 2    JS(I,1)=0.0
C
C-----COMPUTE FLUXES FROM POINT 2 TO POINT NETA-1 - - - - - - - - - - -
C
      DO100N=2,NM1
      T=TT(N)
      P=PI(N)
      THETA=RO(N)/DTIL
C-----DETERMINE WHICH SPECIES ARE PRESENT IN SIGNIFICANT AMOUNTS....
C
```

```
      NS=0
      DO25I=1,NSP
      JS(I,N)=0.0
      IF(Y(I,N).LT..1E-(5)GOTO25
      NS=NS+1
      L(NS)=I
 25   CONTINUE
      NSM1=NS-1
C
C-----COMPUTE B-VECTOR,IF GRADIENTS ARE LESS THAN 1.0E-8, SET FLUXES TO
C     ZERO AND ADVANCE TO NEXT POINT IN FLOW-FIELD....
C
      CALL FGH(N,F,G,H)
      DO3M=1,NS
      I=L(M)
      B(M,1)=DY(I,N)*THETA
 3    CONTINUE
      B(NS,1)=0.0
C
C-----EVALUATE BINARY COEFFICIENTS, D(I,J)....
C
      DO5 I=1,NSP
      DO5 J=I,NSP
      S2=((SIG(I)+SIG(J))*.5)**2
      E=SQRT(EOK(I)*EOK(J))
      TS=T/E
      O=1.061/TS**.156
      M12=SQRT((SMW(I)+SMW(J))/(2.*SMW(I)*SMW(J)))
      T32=T**1.5
      D(I,J)=28.28E-07*T32*M12/(P*S2*O*UINF*RAD)
 5    D(J,I)=D(I,J)
C
C-----COMPUTE A-MATRIX....
C
      DO10II=1,NSM1
      I=L(II)
```

```
      A(II,II)=0.0
      DO10JJ=1,NS
      J=L(JJ)
      IF(I.EQ.J)GOTO10
      A(II,JJ)=Y(J,N)*Y(I,N)/D(I,J)
      A(II,II)=A(II,II) - A(II,JJ)
 10   CONTINUE
      DO45JJ=1,NS
      J=L(JJ)
 45   A(NS,JJ)=Y(J,N)*SMW(J)
C
      CALL MATINV(A,NS ,B,1,NMAX)
C
      DO50II=1,NS
      I=L(II)
 50   JS(I,N)=B(II,1)*Y(I,N)*SMW(I)*RO(N)/AMW(N)
 100  CONTINUE
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      IF(NDBUG.LT.2)GOTO200
 101  FORMAT(1H1,' DIFFUSION FLUXES'/'  ETA ',2X,10(5X,A4,3X))
 102  FORMAT(1X,F6.4,10E12.4)
 103  FORMAT(1H1)
      PRINT 101,(SP(I),I=1,10)
      DO110N=1,NETA
      NCP=10
      IF(NSP.LT.10)NCP=NSP
 110  PRINT 102,ET(N),(JS(I,N),I=1,NCP)
      IF(NSP.LE.10)GOTO130
      PRINT 101,(SP(I),I=11,NSP)
      DO120N=1,NETA
 120  PRINT 102,ET(N),(JS(I,N),I=11,NSP)
 130  PRINT 103
 200  RETURN
      END
```

```
C
      SUBROUTINE EFLUX
C
C-------   CONVERTS MASS FLUXES TO ELEMENTAL BASIS
C
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON /FRSTRM/ U INF, RINF, UINF2, P , RE, LXI, ITM, IEM,NETA
      COMMON/WT/SMW(20),AWT(5)
      COMMON/EQ2/AA(20,5)
      COMMON /MCD1/JS(20,200),JE(5,200)
      REAL JS, JE
      DO15N=1,NETA
      DO10J=1,NE
      JE(J,N)=0.0
      DO10I=1,NSP
   10 JE(J,N)=JE(J,N) + AA(I,J)*AWT(J)*JS(I,N)/SMW(I)
   15 CONTINUE
      RETURN
      END
```

```
C
      SUBROUTINE DIJ
      COMMON/SP1/SS,TOL,NDBUG
      COMMON /VEL/FF(200),FC(200),ZZ(200),VV(200)
      COMMON /MCD1/JS(20,200),JE(5,200)
      COMMON/NUMBER/NSP,NNS,NE,NC
      COMMON /FRSTRM/ U INF, RINF, UINF2,RAD, RE, LXI, ITM, IEM,NETA
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /YL/ ET(200),YOND(200)
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON /DIF/D(5,200)
      DIMENSION DCDE(5)
      REAL*4 DCDE
      REAL*4 JS,JE
      NM1=NETA-1
      DO10J=1,NE
      JE(J,1)=0.0
   10 JE(J,NETA)=0.0
      DO40N=2,NM1
      RV=RO(N)*VV(N)
      CALL FGH(N,F1,G1,H1)
      DO30J=1,NE
      DNEW = 1.0E-6
      IF(ABS(JE(J,N)/RV).LE..01)GOTO25
      DCDE(J)  =CC(J,N+1)*F1 + CC(J,N)*G1 + CC(J,N-1)*H1
      IF(ABS(DCDE(J)).LE.1.E-3)GOTO25
      DNEW = -JE(J,N)*DTIL/(RO(N)*RO(N)*DCDE(J))
      IF(DNEW.LE.0.0)DNEW=1.0E-6
   25 D(J,N)=D(J,N)*.3 + DNEW*.7
   30 CONTINUE
      IF(NDBUG.LT.2)GOTO40
      PRINT 101,ET(N),(JE(J,N),DCDE(J),D(J,N),J=1,NE)
   40 CONTINUE
      RETURN
  101 FORMAT(F6.3,5(1X,3E8.2))
      END
```

```
      SUBROUTINE COMP(ITYPE,NSP,NETA)
      COMMON/PROF1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /WT/SMW(20),AWT(5)
      IF(ITYPE.EQ.1)GOTO20
C
C-----CONVERT MOLE FRACTIONS TO MASS FRACTIONS....
C
      DO10N=1,NETA
      DO10I=1,NSP
 10   C(I,N)=C(I,N)*SMW(I)/AMW(N)
      ITYPE=1
      RETURN
C
C-----CONVERT MASS FRACTIONS TO MOLE FRACTIONS....
C
 20   DO30N=1,NETA
      DO30I=1,NSP
 30   C(I,N)=C(I,N)*AMW(N)/SMW(I)
      ITYPE=2
      RETURN
      END
```

```
      SUBROUTINE LRAD4
C
C   **   **   PUNCH PROGRAM FOR LRAD4 DATA   **   **   **   **
C
      COMMON/TITL/TITLE(20)
      COMMON/ID/SP(20),EL(5)
      COMMON/WT/SMW(20),AWT(5)
      COMMON /YL/ ET(200),YOND(200)
      COMMON /DEL/ DELTA,DTIL,DTILS
      COMMON/PROP1/PI(200),RO(200),TT(200),AMW(200),C (20,200),CC(5,200)
      COMMON /FRSTRM/ U INF, RINF, UINF2, R , RE, LXI, ITM, IEM, NETA
      DIMENSION SNAME(12),Y(200)
      DATA SNAME/'O2    ','N2    ','O     ','N     ','E-    ','C     ',
     X           'H2    ','C2    ','H2    ','CO    ','C3    ','C2H   '/
      MF=0
      NS=12
      LINES=1
      IDG=1
      IEZ=0
      XMOL=1.0
C
C-----PUNCH HEADER, CONTROL PARAMETERS, FLOW-FIELD PARAMETERS, AND
C     PROFILES....
C
      WRITE(6,100)TITLE
      WRITE(7,100)TITLE
      WRITE(6,101)NETA,MF,NS,LINES,IDG,IEZ
      WRITE(7,101)NETA,MF,NS,LINES,IDG,IEZ
      WRITE(6,105)R,DELTA,DTIL,XMOL
      WRITE(7,105)R,DELTA,DTIL,XMOL
      WRITE(6,105)(TT(I),I=1,NETA)
      WRITE(7,105)(TT(I),I=1,NETA)
      WRITE(6,105)(YOND(I),I=1,NETA)
      WRITE(7,105)(YOND(I),I=1,NETA)
      WRITE(6,105)(ET(I),I=1,NETA)
      WRITE(7,105)(ET(I),I=1,NETA)
```

```
C
      DO20I=1,NS
C
C-----SEARCH FOR SPECIES CORRESPONDING TO LRAD4 LISTING--THEN
C     SET INDEX TO PROPER VALUE....
C
      L=0
      DO15K=1,20
      IF(SP(K).EQ.SNAME(I))L=K
 15   CONTINUE
      IF(L.EQ.0)GOTO20
C
      WRITE(6,104)I,SP(L)
      WRITE(7,104)I,SP(L)
C
C-----COMPUTE AND PUNCH NUMBER DENSITIES FOR THOSE SPECIES INCLUDED
C     IN THE LRAD4 RADIATION PROGRAM....
C
      DO10N=1,NETA
 10   Y(N)=(C(L,N)*AMW(N)/SMW(L))*7.336E21*PI(N)/TT(N)
C
      WRITE(6,105)(Y(N),N=1,NETA)
      WRITE(7,105)(Y(N),N=1,NETA)
 20   CONTINUE
C
      RETURN
 100  FORMAT(20A4)
 101  FORMAT(6I5)
 104  FORMAT(I5,2X,A4)
 105  FORMAT(6E12.5)
      END
```

```
SLAB  P=0.1,BLOWING RATE=0.05 7-2-585
   2   50   20          5   20
0.1000E-110.5000E 050.5384E-010.9000E 010.2847E-050.5364E-010.3946E-01
 0.0          0.5000E-02  0.1000E-01  0.1500E-01  0.2000E-01  0.2312E-01
 0.2625E-01   0.2937E-01  0.3250E-01  0.3562E-01  0.3875E-01  0.4500E-01
 0.5375E-01   0.6250E-01  0.7125E-01  0.8000E-01  0.8500E-01  0.9250E-01
 0.1000E 00   0.1100E 00  0.1200E 00  0.1300E 00  0.1400E 00  0.1500E 00
 0.1600E 00   0.1700E 00  0.1800E 00  0.2000E 00  0.2100E 00  0.2200E 00
 0.2300E 00   0.2400E 00  0.2600E 00  0.2800E 00  0.3000E 00  0.3300E 00
 0.3500E 00   0.3800E 00  0.4200E 00  0.4400E 00  0.4800E 00  0.5000E 00
 0.5400E 00   0.5600E 00  0.5800E 00  0.6200E 00  0.6400E 00  0.6800E 00
 0.7000E 00   0.7400E 00  0.7600E 00  0.8000E 00  0.8200E 00  0.8600E 00
 0.8800E 00   0.9200E 00  0.9400E 00  0.9800E 00  0.1000E 01
 0.0          0.1336E-02  0.2754E-02  0.4264E-02  0.5874E-02  0.6935E-02
 0.8043E-02   0.9200E-02  0.1041E-01  0.1167E-01  0.1299E-01  0.1578E-01
 0.2003E-01   0.2465E-01  0.2959E-01  0.3484E-01  0.3798E-01  0.4291E-01
 0.4813E-01   0.5561E-01  0.6369E-01  0.7231E-01  0.8138E-01  0.9081E-01
 0.1006E 00   0.1105E 00  0.1207E 00  0.1412E 00  0.1514E 00  0.1616E 00
 0.1717E 00   0.1816E 00  0.2011E 00  0.2201E 00  0.2387E 00  0.2659E 00
 0.2840E 00   0.3111E 00  0.3481E 00  0.3670E 00  0.4057E 00  0.4256E 00
 0.4660E 00   0.4866E 00  0.5075E 00  0.5499E 00  0.5715E 00  0.6152E 00
 0.6375E 00   0.6826E 00  0.7055E 00  0.7521E 00  0.7757E 00  0.8237E 00
 0.8480E 00   0.8975E 00  0.9226E 00  0.9739E 00  0.1000E 01
 0.3450E 04   0.3523E 04  0.3599E 04  0.3680E 04  0.3765E 04  0.3821E 04
 0.3880E 04   0.3942E 04  0.4006E 04  0.4073E 04  0.4144E 04  0.4295E 04
 0.4528E 04   0.4780E 04  0.5048E 04  0.5329E 04  0.5494E 04  0.5752E 04
 0.6028E 04   0.6426E 04  0.6852E 04  0.7280E 04  0.7688E 04  0.8066E 04
 0.8407E 04   0.8707E 04  0.8967E 04  0.9369E 04  0.9526E 04  0.9660E 04
 0.9776E 04   0.9880E 04  0.1007E 05  0.1025E 05  0.1043E 05  0.1071E 05
 0.1089E 05   0.1114E 05  0.1141E 05  0.1153E 05  0.1170E 05  0.1177E 05
 0.1189E 05   0.1194E 05  0.1199E 05  0.1209E 05  0.1214E 05  0.1223E 05
 0.1227E 05   0.1236E 05  0.1240E 05  0.1249E 05  0.1253E 05  0.1262E 05
 0.1267E 05   0.1276E 05  0.1281E 05  0.1292E 05  0.1300E 05
 0.9895E-01   0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01   0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01   0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
```

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 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01  0.9895E-01
 0.2561E 02  0.2715E 02  0.2885E 02  0.3070E 02  0.3275E 02  0.3412E 02
 0.3558E 02  0.3710E 02  0.3867E 02  0.4028E 02  0.4189E 02  0.4498E 02
 0.4867E 02  0.5155E 02  0.5390E 02  0.5590E 02  0.5686E 02  0.5834E 02
 0.5993E 02  0.6179E 02  0.6251E 02  0.6159E 02  0.5922E 02  0.5555E 02
 0.5060E 02  0.4437E 02  0.3691E 02  0.1880E 02  0.8544E 01 -0.2259E 01
-0.1343E 02 -0.2485E 02 -0.4804E 02 -0.7181E 02 -0.9450E 02 -0.1294E 03
-0.1547E 03 -0.1981E 03 -0.2675E 03 -0.3069E 03 -0.3948E 03 -0.4422E 03
-0.5438E 03 -0.5982E 03 -0.6550E 03 -0.7763E 03 -0.8412E 03 -0.9786E 03
-0.1052E 04 -0.1207E 04 -0.1290E 04 -0.1464E 04 -0.1557E 04 -0.1752E 04
-0.1856E 04 -0.2076E 04 -0.2194E 04 -0.2446E 04 -0.2591E 04
 0.5259E 01  0.4960E 01  0.4667E 01  0.4381E 01  0.4102E 01  0.3932E 01
 0.3767E 01  0.3607E 01  0.3454E 01  0.3309E 01  0.3175E 01  0.2939E 01
 0.2685E 01  0.2496E 01  0.2343E 01  0.2206E 01  0.2133E 01  0.2021E 01
 0.1903E 01  0.1752E 01  0.1628E 01  0.1539E 01  0.1472E 01  0.1421E 01
 0.1381E 01  0.1353E 01  0.1334E 01  0.1327E 01  0.1334E 01  0.1347E 01
 0.1363E 01  0.1382E 01  0.1421E 01  0.1454E 01  0.1488E 01  0.1513E 01
 0.1515E 01  0.1498E 01  0.1456E 01  0.1432E 01  0.1386E 01  0.1366E 01
 0.1331E 01  0.1316E 01  0.1301E 01  0.1273E 01  0.1259E 01  0.1234E 01
 0.1221E 01  0.1197E 01  0.1185E 01  0.1161E 01  0.1149E 01  0.1127E 01
 0.1115E 01  0.1091E 01  0.1079E 01  0.1052E 01  0.1035E 01
 C+       12.011      15.000        30.6        0.0          0.0          10000
0.2528E 010.4869E-05-.7626E-080.1134E-11-.3475E-160.2168E 060.4139E 01  C+      B3
0.2609E 01-.1393E-030.5959E-07-.1037E-100.6345E-150.2168E 060.3709E 01  C+      B2
 H         1.008       2.708        37.0   1.7168E-02      0.0          01000
0.3934E 01-.1776E-020.6013E-06-.7819E-100.3482E-140.2547E 05-.8598E 01  H       B3
0.2599E 01-.8243E-060.6421E-09-.1720E-120.1457E-150.2547E 05-.4612E 00  H       B2
 N+       14.0[illegible]8     14.93        71.4        0.0   3.8688E-01          00100
0.2499E 01-.3725E-050.1147E-07-.1102E-110.3078E-160.2254E 060.4950E 01  N+      B3
0.2727E 01-.2820E-030.1105E-06-.1551E-100.7847E-150.2254E 060.3645E 01  N+      B2
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 O+       16.000      14.22      106.7       0.0    7.2149E-02       00010
0.2944E 01-.4108E-030.9156E-07-.5848E-110.1190E-150.1879E 060.1750E 01  O+      B3
0.2491E 010.2762E-04-.1881E-070.3807E-11-.1028E-150.1879E 060.4424E 01  O+      B2
 E-     5.486E-4    14.93       71.4  7.5326E-10 1.770E-05       00001
0.2508E 01-.6332E-050.1364E-08-.1094E-120.2934E-17-.7450E 03-.1208E 02  E-      B3
0.2500E 010.3440E-06-.1954E-090.3937E-13-.2573E-17-.7450E 03-.1173E 02  E-      B2
 C        12.011      3.365      30.6  1.5893E-03     0.0         10001
0.2141E 010.3219E-03-.5498E-070.3604E-11-.5564E-160.8542E 050.6874E 01  C       B3
0.2612E 01-.2030E-030.1095E-06-.1695E-100.8590E-150.8542E 050.4144E 01  C       B2
 CN       26.019      3.856      75.0  1.8989E-02     0.0         10102
0.3473E 010.7337E-03-.9088E-070.4847E-11-.1018E-150.5420E 050.4152E 01  CN      B3
0.3411E 010.4897E-030.1005E-06-.3473E-100.2361E-140.4745E 050.4746E 01  CN      B2
 CO       28.011      3.690      91.7  2.5784E-01     0.0         10012
0.3366E 010.8027E-03-.1968E-060.1940E-10-.5549E-15-.1434E 050.4263E 01  CO      B3
0.3254E 010.9698E-03-.2647E-060.3037E-10-.1177E-14-.1434E 050.4875E 01  CO      B2
 C2       24.022      3.913      78.8  4.2760E-03     0.0         20002
0.4026E 010.4857E-03-.7026E-070.4666E-11-.1142E-150.9787E 050.1090E 01  C2      B3
0.4443E 01-.2885E-030.3036E-06-.6244E-100.3915E-140.9787E 05-.1090E 01  C2      B2
 C2H      25.030      3.880     205.0  1.5543E-01     0.0         21002
0.5307E 010.8966E-03-.1378E-060.9251E-11-.2278E-150.5809E 05-.5288E 01  C2H     B3
0.3485E 010.3563E-02-.1237E-050.1856E-09-.1013E-130.5809E 050.4784E 01  C2H     B2
 C2H2     26.038      4.033     231.8  8.5629E-02     0.0         22002
0.6789E 010.1503E-02-.2295E-060.1534E-10-.3763E-150.2590E 05-.1539E 02  C2H2    B3
0.3891E 010.5717E-02-.1957E-050.2931E-09-.1585E-130.2590E 050.6520E 00  C2H2    B2
 C3       36.033      4.450     128.0  2.0563E-02     0.0         30003
0.2213E 02-.1759E-010.5565E-05-.6758E-090.2825E-130.9423E 05-.1021E 03  C3      B3
0.4002E 010.3541E-02-.1316E-050.2064E-09-.1144E-130.9423E 050.2020E 01  C3      B2
 C3H      37.041      4.600     356.0  1.7822E-01     0.0         31003
.3964709E1.620030E-2-.22655E-5.371712E-9-.2262E-13.6283285E5.3467072E1  C3H    *D2
.3964709E1.620030E-2-.22655E-5.371712E-9-.2262E-13.6283285E5.3467072E1  C3H    *D2
 C4H      49.052      5.210     504.0  1.6777E-01     0.0         41004
.5873679E1.740338E-2-.27289E-5.443720E-9-.2637E-13.7605163E5-.401004E1  C4H    *D2
.5873679E1.740338E-2-.27289E-5.443720E-9-.2637E-13.7605163E5-.401004E1  C4H    *D2
 HCN      27.027      3.630     569.1  4.1142E-02     0.0         11102
3.653803E03.44363E-3-1.2585E-62.1692E-10-1.430E-141.442180E42.372602E0  HCN    *M3
3.653803E03.44363E-3-1.2585E-62.1692E-10-1.430E-141.442180E42.372602E0  HCN    *M2
```

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H2        2.016     2.827     59.7   3.2934E-02    0.0          02000
0.3363E 010.4656E-03-.5127E-070.2802E-11-.4905E-16-.1018E 04-.3716E 01  H2     B3
0.3358E 010.2794E-030.9372E-07-.2948E-100.2141E-14-.1018E 04-.3548E 01  H2     B2
N        14.008      7.94     71.4      0.0   3.9086E-01      00101
0.2746E 01-.3909E-030.1338E-06-.1191E-100.3369E-150.5609E 050.2872E 01  N      B3
0.2474E 010.9097E-04-.7814E-070.2218E-10-.1489E-140.5609E 050.4300E 01  N      B2
O        16.000      7.99    106.7      0.0   1.5007E-01      00011
0.2548E 01-.5952E-040.2701E-07-.2798E-110.9380E-160.2915E 050.5049E 01  O      B3
0.2670E 01-.1970E-030.7193E-07-.8901E-110.4002E-150.2915E 050.4504E 01  O      B2
N2       28.016      3.798     71.4  1.8435E-02 1.360E-05      00202
0.3727E 010.4684E-03-.1140E-060.1154E-10-.3293E-15-.1043E 040.1294E 01  N2     B3
0.3221E 010.9878E-03-.2907E-060.3938E-10-.2000E-14-.1043E 040.4326E 01  N2     B2
O2       32.000      3.467    106.7      0.0                   00022
0.3721E 010.4254E-03-.2835E-070.6050E-12-.5186E-17-.1044E 040.3254E 01  O2     B3
0.3316E 010.1151E-02-.3726E-060.6186E-10-.3665E-14-.1044E 040.5393E 01  O2     B2
 0.810E-07
```

SLAB P=0.1,BLOWING RATE=0.05 7-2-585

NETA	NSP	UINF	DTIL	RAD	RINF	RZB	DELTA
59	20	0.500E 05	0.538E-01	0.900E 01	0.285E-05	0.536E-01	0.395E-01

SPECIES	SMW	SIGMA	EOK	CWALL	CSHOCK	A(I,J)
C+	12.011	15.000	30.6	0.0	0.0	10000
H	1.008	2.708	37.0	0.01717	0.0	01000
N+	14.008	14.930	71.4	0.0	0.38688	00100
O+	16.000	14.220	106.7	0.0	0.07215	00010
E-	0.001	14.930	71.4	0.00000	0.00002	00001
C	12.011	3.385	30.6	0.00159	0.0	10001
CN	26.019	3.856	75.0	0.01899	0.0	10102
CO	28.011	3.690	91.7	0.25784	0.0	10012
C2	24.022	3.913	78.8	0.00428	0.0	20002
C2H	25.030	3.880	205.0	0.15543	0.0	21002
C2H2	26.038	4.033	231.8	0.08563	0.0	22002
C3	36.033	4.450	128.0	0.02056	0.0	30003
C3H	37.041	4.600	356.0	0.17822	0.0	31003
C4H	49.052	5.210	504.0	0.16777	0.0	41004
HCN	27.027	3.630	569.1	0.04114	0.0	11102
H2	2.016	2.827	59.7	0.03293	0.0	02000
N	14.008	7.940	71.4	0.0	0.39086	00101
O	16.000	7.990	106.7	0.0	0.15007	00011
N2	28.016	3.798	71.4	0.01843	0.00001	00202
O2	32.000	3.467	106.7	0.0	0.0	00022

SPECIES	THERMO-CONSTANTS A-G							RANGE
C+	0.2609E 01	-0.1393E-03	0.5959E-07	-0.1037E-10	0.6345E-15	0.2168E 06	0.3709E 01	LOW RANGE
	0.2528E 01	0.4869E-05	-0.7026E-08	0.1134E-11	-0.3476E-16	0.2168E 06	0.4139E 01	HIGH RANGE
H	0.2500E 01	-0.8243E-06	0.6421E-09	-0.1720E-12	0.1457E-16	0.2547E 05	-0.4612E 00	LOW RANGE
	0.3934E 01	-0.1776E-02	0.6013E-06	-0.7819E-10	0.3482E-14	0.2547E 05	-0.8598E 01	HIGH RANGE
N+	0.2727E 01	-0.2820E-03	0.1105E-06	-0.1551E-10	0.7847E-15	0.2254E 06	0.3645E 01	LOW RANGE
	0.2499E 01	-0.3725E-05	0.1147E-07	-0.1102E-11	0.3078E-16	0.2254E 06	0.4950E 01	HIGH RANGE
O+	0.2491E 01	0.2762E-04	-0.1881E-07	0.3807E-11	-0.1028E-15	0.1879E 06	0.4424E 01	LOW RANGE
	0.2944E 01	-0.4108E-03	0.9156E-07	-0.5848E-11	0.1190E-15	0.1879E 06	0.1750E 01	HIGH RANGE
E-	0.2500E 01	0.3440E-06	-0.1954E-09	0.3937E-13	-0.2573E-17	-0.7450E 03	-0.1173E 02	LOW RANGE
	0.2508E 01	-0.6332E-05	0.1364E-08	-0.1094E-12	0.2934E-17	-0.7450E 03	-0.1208E 02	HIGH RANGE
C	0.2612E 01	-0.2030E-03	0.1095E-06	-0.1695E-10	0.8590E-15	0.8542E 05	0.4144E 01	LOW RANGE
	0.2141E 01	0.3219E-03	-0.5498E-07	0.3604E-11	-0.5564E-16	0.8542E 05	0.6874E 01	HIGH RANGE
CN	0.3411E 01	0.4897E-03	0.1005E-06	-0.3473E-10	0.2361E-14	0.4745E 05	0.4746E 01	LOW RANGE
	0.3473E 01	0.7337E-03	-0.9088E-07	0.4847E-11	-0.1018E-15	0.5420E 05	0.4152E 01	HIGH RANGE
CO	0.3254E 01	0.9698E-03	-0.2647E-06	0.3037E-10	-0.1177E-14	-0.1434E 05	0.4875E 01	LOW RANGE
	0.3366E 01	0.8027E-03	-0.1968E-06	0.1940E-10	-0.5549E-15	-0.1434E 05	0.4263E 01	HIGH RANGE
C2	0.4443E 01	-0.2885E-03	0.3036E-06	-0.6244E-10	0.3915E-14	0.9787E 05	-0.1090E 01	LOW RANGE
	0.4026E 01	0.4857E-03	-0.7026E-07	0.4666E-11	-0.1142E-15	0.9787E 05	0.1090E 01	HIGH RANGE
C2H	0.3485E 01	0.3563E-02	-0.1237E-05	0.1866E-09	-0.1013E-13	0.5809E 05	0.4784E 01	LOW RANGE
	0.5307E 01	0.8966E-03	-0.1378E-06	0.9251E-11	-0.2278E-15	0.5809E 05	-0.5288E 01	HIGH RANGE
C2H2	0.3891E 01	0.5717E-02	-0.1957E-05	0.2931E-09	-0.1585E-13	0.2590E 05	0.6520E 00	LOW RANGE
	0.6789E 01	0.1503E-02	-0.2295E-06	0.1534E-10	-0.3763E-15	0.2590E 05	-0.1539E 02	HIGH RANGE
C3	0.4002E 01	0.3541E-02	-0.1318E-05	0.2064E-09	-0.1144E-13	0.9423E 05	0.2020E 01	LOW RANGE
	0.2213E 02	-0.1759E-01	0.5565E-05	-0.6756E-09	0.2825E-13	0.9423E 05	-0.1021E 03	HIGH RANGE
C3H	0.3965E 01	0.6200E-02	-0.2265E-05	0.3717E-09	-0.2262E-13	0.6283E 05	0.3467E 01	LOW RANGE
	0.3965E 01	0.6200E-02	-0.2265E-05	0.3717E-09	-0.2262E-13	0.6283E 05	0.3467E 01	HIGH RANGE
C4H	0.5874E 01	0.7403E-02	-0.2729E-05	0.4437E-09	-0.2637E-13	0.7605E 05	-0.4010E 01	LOW RANGE
	0.5874E 01	0.7403E-02	-0.2729E-05	0.4437E-09	-0.2637E-13	0.7605E 05	-0.4010E 01	HIGH RANGE
HCN	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	LOW RANGE
	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	HIGH RANGE
H2	0.3358E 01	0.2794E-03	0.9372E-07	-0.2948E-10	0.2141E-14	-0.1018E 04	-0.3548E 01	LOW RANGE
	0.3363E 01	0.4656E-03	-0.5127E-07	0.2802E-11	-0.4905E-16	-0.1018E 04	-0.3716E 01	HIGH RANGE
N	0.2474E 01	0.9097E-04	-0.7814E-07	0.2218E-10	-0.1489E-14	0.5609E 05	0.4300E 01	LOW RANGE
	0.2746E 01	-0.3909E-03	0.1338E-06	-0.1191E-10	0.3369E-15	0.5609E 05	0.2872E 01	HIGH RANGE
O	0.2670E 01	-0.1970E-03	0.7193E-07	-0.8901E-11	0.4002E-15	0.2915E 05	0.4504E 01	LOW RANGE
	0.2548E 01	-0.5952E-04	0.2701E-07	-0.2798E-11	0.9380E-16	0.2915E 05	0.5049E 01	HIGH RANGE
N2	0.3221E 01	0.9878E-03	-0.2907E-06	0.3938E-10	-0.2000E-14	-0.1043E 04	0.4326E 01	LOW RANGE
	0.3727E 01	0.4684E-03	-0.1140E-06	0.1154E-10	-0.3293E-15	-0.1043E 04	0.1294E 01	HIGH RANGE
O2	0.3316E 01	0.1151E-02	-0.3726E-06	0.6186E-10	-0.3666E-14	-0.1044E 04	0.5393E 01	LOW RANGE
	0.3721E 01	0.4254E-03	-0.2835E-07	0.6050E-12	-0.5186E-17	-0.1044E 04	0.3254E 01	HIGH RANGE

REVISED ETA DISTRIBUTION....

0.0	0.5000E-02	0.7500E-02	0.1000E-01	0.1250E-01	0.1500E-01	0.1750E-01	0.2000E-01	0.2312E-01	0.2625E-01
0.2937E-01	0.3250E-01	0.3562E-01	0.3875E-01	0.4083E-01	0.4292E-01	0.4500E-01	0.4719E-01	0.4937E-01	0.5156E-01
0.5375E-01	0.5594E-01	0.5812E-01	0.6031E-01	0.6250E-01	0.6469E-01	0.6687E-01	0.6906E-01	0.7125E-01	0.7344E-01
0.7562E-01	0.7781E-01	0.8000E-01	0.8167E-01	0.8333E-01	0.8500E-01	0.8667E-01	0.8875E-01	0.9062E-01	0.9250E-01
0.9437E-01	0.9625E-01	0.9812E-01	0.1000E 00	0.1017E 00	0.1033E 00	0.1050E 00	0.1067E 00	0.1083E 00	0.1100E 00
0.1117E 00	0.1133E 00	0.1150E 00	0.1167E 00	0.1183E 00	0.1200E 00	0.1217E 00	0.1233E 00	0.1250E 00	0.1267E 00
0.1283E 00	0.1300E 00	0.1317E 00	0.1333E 00	0.1350E 00	0.1367E 00	0.1383E 00	0.1400E 00	0.1417E 00	0.1433E 00
0.1450E 00	0.1467E 00	0.1483E 00	0.1500E 00	0.1520E 00	0.1540E 00	0.1560E 00	0.1580E 00	0.1600E 00	0.1620E 00
0.1640E 00	0.1660E 00	0.1680E 00	0.1700E 00	0.1725E 00	0.1750E 00	0.1775E 00	0.1800E 00	0.1833E 00	0.1867E 00
0.1900E 00	0.1933E 00	0.1967E 00	0.2000E 00	0.2033E 00	0.2067E 00	0.2100E 00	0.2150E 00	0.2200E 00	0.2250E 00
0.2300E 00	0.2350E 00	0.2400E 00	0.2467E 00	0.2533E 00	0.2600E 00	0.2667E 00	0.2733E 00	0.2800E 00	0.2867E 00
0.2933E 00	0.3000E 00	0.3075E 00	0.3150E 00	0.3225E 00	0.3300E 00	0.3367E 00	0.3433E 00	0.3500E 00	0.3575E 00
0.3650E 00	0.3725E 00	0.3800E 00	0.3900E 00	0.4000E 00	0.4100E 00	0.4200E 00	0.4300E 00	0.4400E 00	0.4533E 00
0.4667E 00	0.4800E 00	0.5000E 00	0.5200E 00	0.5400E 00	0.5600E 00	0.5800E 00	0.6000E 00	0.6200E 00	0.6400E 00
0.6600E 00	0.6800E 00	0.7000E 00	0.7200E 00	0.7400E 00	0.7600E 00	0.7800E 00	0.8000E 00	0.8200E 00	0.8400E 00
0.8600E 00	0.8800E 00	0.9000E 00	0.9200E 00	0.9400E 00	0.9600E 00	0.9800E 00	0.9900E 00	0.1000E 01	

NETA=159

MULTICOMPONENT SOLUTION CONVERGED IN 5 ITERATIONS

ETA	CARBON	HYDROGEN	NITROGEN	OXYGEN	ELECTRON	T(OK)	VELOCITY	Y/C	DENSITY
	************** ELEMENTAL MASS FRACTIONS **************								
0.0	0.7298E 00	0.7273E-01	0.5002E-01	0.1473E 00	0.4034E-04	0.3450E 04	0.5120E-03	0.0	0.5109E 01
0.0050	0.7298E 00	0.7272E-01	0.5003E-01	0.1473E 00	0.4034E-04	0.3523E 04	0.5436E-03	0.1330E-02	0.4807E 01
0.0100	0.7298E 00	0.7270E-01	0.5004E-01	0.1473E 00	0.4034E-04	0.3597E 04	0.5772E-03	0.2754E-02	0.4512E 01
0.0150	0.7297E 00	0.7268E-01	0.5005E-01	0.1473E 00	0.4034E-04	0.3680E 04	0.6143E-03	0.4264E-02	0.4223E 01
0.0200	0.7297E 00	0.7266E-01	0.5006E-01	0.1473E 00	0.4034E-04	0.3766E 04	0.6554E-03	0.5874E-02	0.3938E 01
0.0231	0.7297E 00	0.7264E-01	0.5007E-01	0.1473E 00	0.4034E-04	0.3822E 04	0.6830E-03	0.6935E-02	0.3763E 01
0.0262	0.7297E 00	0.7262E-01	0.5008E-01	0.1473E 00	0.4034E-04	0.3861E 04	0.7120E-03	0.8043E-02	0.3591E 01
0.0294	0.7297E 00	0.7260E-01	0.5009E-01	0.1473E 00	0.4034E-04	0.3943E 04	0.7423E-03	0.9200E-02	0.3425E 01
0.0325	0.7297E 00	0.7258E-01	0.5010E-01	0.1473E 00	0.4034E-04	0.4007E 04	0.7737E-03	0.1041E-01	0.3265E 01
0.0356	0.7297E 00	0.7256E-01	0.5011E-01	0.1473E 00	0.4034E-04	0.4074E 04	0.8056E-03	0.1167E-01	0.3114E 01
0.0387	0.7296E 00	0.7253E-01	0.5013E-01	0.1473E 00	0.4034E-04	0.4145E 04	0.8377E-03	0.1299E-01	0.2973E 01
0.0450	0.7296E 00	0.7248E-01	0.5017E-01	0.1473E 00	0.4034E-04	0.4296E 04	0.8993E-03	0.1578E-01	0.2721E 01
0.0537	0.7295E 00	0.7238E-01	0.5025E-01	0.1473E 00	0.4034E-04	0.4528E 04	0.9730E-03	0.2003E-01	0.2454E 01
0.0625	0.7294E 00	0.7226E-01	0.5037E-01	0.1473E 00	0.4033E-04	0.4780E 04	0.1031E-02	0.2465E-01	0.2261E 01
0.0712	0.7292E 00	0.7213E-01	0.5054E-01	0.1474E 00	0.4033E-04	0.5048E 04	0.1078E-02	0.2959E-01	0.2111E 01
0.0800	0.7290E 00	0.7198E-01	0.5079E-01	0.1474E 00	0.4033E-04	0.5329E 04	0.1118E-02	0.3484E-01	0.1979E 01
0.0850	0.7288E 00	0.7187E-01	0.5099E-01	0.1475E 00	0.4033E-04	0.5494E 04	0.1137E-02	0.3798E-01	0.1909E 01
0.0925	0.7285E 00	0.7165E-01	0.5139E-01	0.1475E 00	0.4033E-04	0.5752E 04	0.1167E-02	0.4291E-01	0.1807E 01
0.1000	0.7280E 00	0.7136E-01	0.5197E-01	0.1477E 00	0.4033E-04	0.6028E 04	0.1199E-02	0.4813E-01	0.1703E 01
0.1100	0.7270E 00	0.7090E-01	0.5326E-01	0.1479E 00	0.4032E-04	0.6426E 04	0.1236E-02	0.5561E-01	0.1561E 01
0.1200	0.7251E 00	0.7031E-01	0.5562E-01	0.1485E 00	0.4032E-04	0.6852E 04	0.1250E-02	0.6369E-01	0.1439E 01
0.1300	0.7215E 00	0.6922E-01	0.6004E-01	0.1494E 00	0.4031E-04	0.7280E 04	0.1232E-02	0.7231E-01	0.1348E 01
0.1400	0.7146E 00	0.6718E-01	0.6801E-01	0.1512E 00	0.4029E-04	0.7688E 04	0.1184E-02	0.8138E-01	0.1276E 01
0.1500	0.7015E 00	0.6403E-01	0.8202E-01	0.1544E 00	0.4025E-04	0.8066E 04	0.1111E-02	0.9081E-01	0.1227E 01
0.1600	0.6788E 00	0.5992E-01	0.1056E 00	0.1587E 00	0.4019E-04	0.8406E 04	0.1012E-02	0.1006E 00	0.1193E 01
0.1700	0.6419E 00	0.5492E-01	0.1427E 00	0.1640E 00	0.4009E-04	0.8706E 04	0.8870E-03	0.1105E 00	0.1191E 01
0.1800	0.5876E 00	0.4923E-01	0.1962E 00	0.1703E 00	0.3994E-04	0.8966E 04	0.7376E-03	0.1207E 00	0.1200E 01
0.2000	0.4335E 00	0.3695E-01	0.3460E 00	0.1843E 00	0.3948E-04	0.9368E 04	0.3755E-03	0.1412E 00	0.1269E 01
0.2100	0.3465E 00	0.3106E-01	0.4293E 00	0.1911E 00	0.3922E-04	0.9525E 04	0.1703E-03	0.1514E 00	0.1323E 01
0.2200	0.2633E 00	0.2568E-01	0.5099E 00	0.1973E 00	0.3897E-04	0.9658E 04	-0.4578E-04	0.1616E 00	0.1385E 01
0.2300	0.1900E 00	0.2088E-01	0.5805E 00	0.2029E 00	0.3875E-04	0.9775E 04	-0.2690E-03	0.1717E 00	0.1451E 01
0.2400	0.1298E 00	0.1667E-01	0.6388E 00	0.2077E 00	0.3857E-04	0.9879E 04	-0.4972E-03	0.1816E 00	0.1517E 01
0.2600	0.5056E-01	0.9887E-02	0.7176E 00	0.2150E 00	0.3833E-04	0.1007E 05	-0.9614E-03	0.2011E 00	0.1634E 01
0.2800	0.1558E-01	0.4852E-02	0.7558E 00	0.2196E 00	0.3822E-04	0.1025E 05	-0.1435E-02	0.2201E 00	0.1714E 01
0.3000	0.4375E-02	0.1521E-02	0.7712E 00	0.2215E 00	0.3817E-04	0.1043E 05	-0.1890E-02	0.2387E 00	0.1745E 01
0.3300	0.4118E-03	0.1431E-03	0.7771E 00	0.2221E 00	0.3815E-04	0.1071E 05	-0.2589E-02	0.2659E 00	0.1695E 01
0.3500	0.5233E-04	0.1819E-04	0.7777E 00	0.2222E 00	0.3815E-04	0.1089E 05	-0.3096E-02	0.2840E 00	0.1642E 01
0.3800	0.6882E-06	0.2392E-06	0.7777E 00	0.2222E 00	0.3815E-04	0.1114E 05	-0.3966E-02	0.3111E 00	0.1564E 01
0.4200	0.1148E-09	0.1051E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1141E 05	-0.5355E-02	0.3481E 00	0.1480E 01
0.4400	0.1001E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1153E 05	-0.6145E-02	0.3670E 00	0.1444E 01
0.4800	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1170E 05	-0.7905E-02	0.4057E 00	0.1401E 01
0.5000	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1177E 05	-0.8859E-02	0.4256E 00	0.1371E 01
0.5400	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1189E 05	-0.1089E-01	0.4660E 00	0.1335E 01
0.5600	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1194E 05	-0.1198E-01	0.4866E 00	0.1320E 01
0.5800	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1199E 05	-0.1312E-01	0.5075E 00	0.1305E 01
0.6200	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1209E 05	-0.1555E-01	0.5499E 00	0.1276E 01
0.6400	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1214E 05	-0.1684E-01	0.5715E 00	0.1271E 01
0.6800	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1223E 05	-0.1959E-01	0.6152E 00	0.1244E 01
0.7000	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1227E 05	-0.2106E-01	0.6375E 00	0.1224E 01
0.7400	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1236E 05	-0.2417E-01	0.6826E 00	0.1200E 01
0.7600	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1240E 05	-0.2582E-01	0.7055E 00	0.1196E 01
0.8000	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1249E 05	-0.2931E-01	0.7521E 00	0.1173E 01
0.8200	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1253E 05	-0.3116E-01	0.7757E 00	0.1154E 01
0.8600	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1262E 05	-0.3507E-01	0.8237E 00	0.1131E 01
0.8800	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1267E 05	-0.3715E-01	0.8480E 00	0.1126E 01
0.9200	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1276E 05	-0.4156E-01	0.8975E 00	0.1103E 01
0.9400	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1281E 05	-0.4391E-01	0.9226E 00	0.1083E 01
0.9800	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1292E 05	-0.4896E-01	0.9739E 00	0.1057E 01
1.0000	0.1000E-09	0.1000E-09	0.7778E 00	0.2222E 00	0.3815E-04	0.1300E 05	-0.5180E-01	0.1000E 01	0.1039E 01

9

EQUILIBRIUM MASS FRACTIONS

ETA	C+	H	N+	O+	E-	C	CN	CC	C2	C2H
0.0	0.5510E-04	0.4141E-01	0.1155E-10	0.6886E-13	0.1117E-14	0.1434E-01	0.4505E-01	0.2573E 00	0.2751E-01	0.1904E 00
0.0050	0.5507E-05	0.4543E-01	0.4517E-11	0.6291E-14	0.6080E-14	0.2158E-01	0.5084E-01	0.2579E 00	0.3873E-01	0.1892E 00
0.0100	-0.4959E-11	0.4937E-01	-0.3971E-17	-0.5795E-20	0.2720E-11	0.3286E-01	0.5644E-01	0.2578E 00	0.5421E-01	0.1821E 00
0.0150	0.4623E-08	0.5327E-01	0.1247E-14	0.5863E-17	0.2875E-16	0.4907E-01	0.6169E-01	0.2578E 00	0.7373E-01	0.1695E 00
0.0200	0.1839E-06	0.5710E-01	0.4809E-13	0.6528E-15	0.8598E-15	0.7262E-01	0.6641E-01	0.2578E 00	0.5760E-01	0.1507E 00
0.0231	0.5677E-08	0.5930E-01	0.4016E-14	0.2050E-16	0.9294E-17	0.9269E-01	0.6888E-01	0.2578E 00	0.1141E 00	0.1358E 00
0.0262	0.2431E-06	0.6155E-01	0.1581E-12	0.1443E-14	-0.8866E-16	0.1169E 00	0.7103E-01	0.2578E 00	0.1307E 00	0.1192E 00
0.0294	0.6043E-09	0.6357E-01	0.3589E-15	0.2521E-17	0.7476E-12	0.1461E 00	0.7277E-01	0.2578E 00	0.1463E 00	0.1015E 00
0.0325	0.8784E-13	0.6542E-01	0.5707E-19	0.6353E-21	0.2964E-09	0.1801E 00	0.7408E-01	0.2579E 00	0.1594E 00	0.8343E-01
0.0356	0.2778E-09	0.6703E-01	0.2406E-15	0.6013E-17	0.1505E-09	0.2193E 00	0.7486E-01	0.2579E 00	0.1678E 00	0.6602E-01
0.0387	-0.8870E-13	0.6840E-01	-0.1321E-18	-0.1764E-20	0.3763E-07	0.2622E 00	0.7514E-01	0.2579E 00	0.1706E 00	0.4994E-01
0.0450	0.2360E-06	0.7040E-01	0.3492E-12	0.6491E-14	0.3220E-07	0.3528E 00	0.7387E-01	0.2579E 00	0.1555E 00	0.2501E-01
0.0537	0.1740E-05	0.7183E-01	0.7644E-11	0.1019E-12	0.3235E-07	0.4632E 00	0.6733E-01	0.2578E 00	0.1040E 00	0.7126E-02
0.0625	0.1050E-04	0.7236E-01	0.9111E-10	0.3724E-11	0.3303E-07	0.5333E 00	0.5540E-01	0.2576E 00	0.5598E-01	0.1693E-02
0.0712	0.2092E-03	0.7241E-01	0.9357E-08	0.6346E-09	0.8921E-08	0.5717E 00	0.4080E-01	0.2567E 00	0.2767E-01	0.3896E-03
0.0800	0.4561E-03	0.7243E-01	0.5052E-07	0.6844E-08	0.1916E-07	0.5944E 00	0.2648E-01	0.2530E 00	0.1352E-01	0.9220E-04
0.0850	0.6866E-03	0.7241E-01	0.1173E-06	0.2436E-07	0.2923E-07	0.6040E 00	0.1962E-01	0.2475E 00	0.9097E-02	0.4190E-04
0.0925	0.1252E-02	0.7233E-01	0.3665E-06	0.1476E-06	0.5377E-07	0.6187E 00	0.1164E-01	0.2292E 00	0.5117E-02	0.1330E-04
0.1000	0.2260E-02	0.7219E-01	0.1017E-05	0.7616E-06	0.9851E-07	0.6386E 00	0.6425E-02	0.1857E 00	0.2959E-02	0.4392E-05
0.1100	0.4930E-02	0.7195E-01	0.3496E-05	0.4604E-05	0.2169E-06	0.6730E 00	0.2746E-02	0.1078E 00	0.1481E-02	0.1056E-05
0.1200	0.1022E-01	0.7157E-01	0.1096E-04	0.1742E-04	0.4523E-06	0.6946E 00	0.1177E-02	0.4271E-01	0.7472E-03	0.2677E-06
0.1300	0.1661E-01	0.7084E-01	0.2713E-04	0.4756E-04	0.7327E-06	0.6951E 00	0.2254E-03	0.1754E-01	0.3854E-03	0.7530E-07
0.1400	0.2803E-01	0.6947E-01	0.7034E-04	0.1067E-03	0.1250E-05	0.6798E 00	0.1298E-03	0.6760E-02	0.2124E-03	0.2457E-07
0.1500	0.4300E-01	0.6692E-01	0.1715E-03	0.2105E-03	0.1922E-05	0.6516E 00	0.8722E-04	0.2959E-02	0.1239E-03	0.9119E-08
0.1600	0.6034E-01	0.6280E-01	0.3992E-03	0.3760E-03	0.2676E-05	0.6110E 00	0.6779E-04	0.1473E-02	0.7571E-04	0.3760E-08
0.1700	0.7742E-01	0.5760E-01	0.8826E-03	0.6163E-03	0.3429E-05	0.5570E 00	0.5885E-04	0.6170E-03	0.4730E-04	0.1664E-08
0.1800	0.9103E-01	0.5162E-01	0.1828E-02	0.9413E-03	0.4087E-05	0.4898E 00	0.5427E-04	0.4520E-03	0.2554E-04	0.7669E-09
0.2000	0.9834E-01	0.3874E-01	0.6113E-02	0.1870E-02	0.4786E-05	0.3309E 00	0.4562E-04	0.2060E-03	0.1032E-04	0.1591E-09
0.2100	0.9182E-01	0.3258E-01	0.9912E-02	0.2504E-02	0.4813E-05	0.2516E 00	0.3873E-04	0.1353E-03	0.5538E-05	0.6724E-10
0.2200	0.8008E-01	0.2691E-01	0.1498E-01	0.3270E-02	0.4666E-05	0.1810E 00	0.3051E-04	0.8727E-04	0.2718E-05	0.2614E-10
0.2300	0.6545E-01	0.2185E-01	0.2135E-01	0.4186E-02	0.4420E-05	0.1228E 00	0.2218E-04	0.5445E-04	0.1209E-05	0.9181E-11
0.2400	0.4989E-01	0.1740E-01	0.2894E-01	0.5260E-02	0.4135E-05	0.7850E-01	0.1479E-04	0.3233E-04	0.4802E-06	0.2842E-11
0.2600	0.2317E-01	0.1020E-01	0.4672E-01	0.7804E-02	0.3694E-05	0.2662E-01	0.5068E-05	0.9481E-05	0.5236E-07	0.1745E-12
0.2800	0.8036E-02	0.4947E-02	0.6446E-01	0.1043E-01	0.3593E-05	0.7123E-02	0.1296E-05	0.2204E-05	0.3700E-08	0.5644E-14
0.3000	0.2435E-02	0.1531E-02	0.8000E-01	0.1279E-01	0.3840E-05	0.1894E-02	0.2967E-06	0.4671E-06	0.2254E-09	0.5747E-16
0.3300	0.2507E-03	0.1457E-03	0.1032E 00	0.1644E-01	0.4698E-05	0.1613E-03	0.1944E-07	0.2776E-07	0.1345E-11	0.4772E-19
0.3500	0.3380E-04	0.1881E-04	0.1194E 00	0.1907E-01	0.5406E-05	0.1940E-04	0.1947E-08	0.2630E-08	0.1703E-13	0.4056E-21
0.3800	0.3617E-04	0.1884E-04	0.1446E 00	0.2326E-01	0.6544E-05	0.1776E-04	0.1286E-08	0.1625E-08	0.1107E-13	0.2089E-20
0.4200	0.3665E-04	0.1887E-04	0.1758E 00	0.2864E-01	0.7955E-05	0.1602E-04	0.7172E-09	0.8550E-09	0.5273E-14	0.2859E-20
0.4400	0.3975E-04	0.1888E-04	0.1906E 00	0.3128E-01	0.8629E-05	0.1531E-04	0.5226E-09	0.6083E-09	0.3128E-14	0.3113E-20
0.4800	0.4087E-04	0.1890E-04	0.2068E 00	0.3421E-01	0.9365E-05	0.1457E-04	0.3492E-09	0.3563E-09	0.1224E-14	0.3360E-20
0.5000	0.4180E-04	0.1890E-04	0.2231E 00	0.3724E-01	0.1011E-04	0.1384E-04	0.2452E-09	0.2700E-09	0.1290E-15	0.3558E-20
0.5400	0.4289E-04	0.1892E-04	0.2406E 00	0.4060E-01	0.1091E-04	0.1315E-04	0.4496E-10	0.4630E-10	0.1042E-15	0.1115E-21
0.5600	0.4338E-04	0.1893E-04	0.2483E 00	0.4209E-01	0.1127E-04	0.1287E-04	0.2369E-10	0.2143E-10	0.6854E-15	0.1134E-21
0.5800	0.4385E-04	0.1893E-04	0.2557E 00	0.4350E-01	0.1161E-04	0.1260E-04	0.2301E-10	0.1893E-10	0.1336E-14	0.1151E-21
0.6200	0.4463E-04	0.1894E-04	0.2714E 00	0.4669E-01	0.1233E-04	0.1202E-04	0.8096E-10	0.6139E-10	0.2735E-14	0.1171E-21
0.6400	0.4463E-04	0.1894E-04	0.2714E 00	0.4669E-01	0.1233E-04	0.1202E-04	0.8096E-10	0.6139E-10	0.2734E-14	0.1171E-21
0.6800	0.4537E-04	0.1895E-04	0.2865E 00	0.4980E-01	0.1303E-04	0.1149E-04	0.7454E-10	0.4866E-10	0.2384E-14	0.1169E-21
0.7000	0.4605E-04	0.1896E-04	0.3003E 00	0.5271E-01	0.1367E-04	0.1103E-04	0.2320E-09	0.2299E-09	0.2057E-14	0.1277E-21
0.7400	0.4671E-04	0.1897E-04	0.3145E 00	0.5577E-01	0.1434E-04	0.1058E-04	0.2149E-09	0.2148E-09	0.1670E-14	0.1379E-21
0.7600	0.4671E-04	0.1897E-04	0.3145E 00	0.5577E-01	0.1434E-04	0.1058E-04	0.2149E-09	0.2148E-09	0.1670E-14	0.1379E-21
0.8000	0.4737E-04	0.1897E-04	0.3290E 00	0.5894E-01	0.1501E-04	0.1014E-04	0.1667E-09	0.1150E-09	0.1334E-14	0.1487E-21
0.8200	0.4802E-04	0.1898E-04	0.3434E 00	0.6222E-01	0.1569E-04	0.9714E-05	0.1074E-09	0.1052E-09	0.8723E-15	0.1601E-21
0.8600	0.4867E-04	0.1899E-04	0.3587E 00	0.6576E-01	0.1641E-04	0.9280E-05	0.7273E-10	0.6511E-10	0.1611E-15	0.3377E-21
0.8800	0.4867E-04	0.1899E-04	0.3587E 00	0.6576E-01	0.1641E-04	0.9280E-05	0.7274E-10	0.6511E-10	0.1612E-15	0.3377E-21
0.9200	0.4934E-04	0.1900E-04	0.3748E 00	0.6960E-01	0.1717E-04	0.8838E-05	0.7594E-10	0.6834E-10	0.1541E-15	0.3829E-21
0.9400	0.5000E-04	0.1901E-04	0.3912E 00	0.7362E-01	0.1795E-04	0.8405E-05	0.7388E-10	0.6056E-10	0.1460E-15	0.4268E-21
0.9800	0.5093E-04	0.1903E-04	0.4103E 00	0.7845E-01	0.1887E-04	0.7946E-05	0.8395E-10	0.7974E-10	0.6288E-15	0.2010E-20
1.0000	0.5148E-04	0.1904E-04	0.4231E 00	0.8180E-01	0.1948E-04	0.7634E-05	0.5947E-10	0.5665E-10	0.4473E-15	0.2187E-20

EQUILIBRIUM MASS FRACTIONS

ETA	C2H2	C3	C3H	C4H	HCN	H2	N	O	N2	C2
0.0	0.1997E-01	0.9429E-01	0.1551E 00	0.1042E 00	0.1851E-01	0.1513E-01	0.5260E-04	0.9715E-07	0.1612E-01	0.3367E-14
0.0050	0.1457E-01	0.1130E 00	0.1382E 00	0.8816E-01	0.1530E-01	0.1249E-01	0.7219E-04	0.1458E-06	0.1465E-01	0.5460E-14
0.0100	0.1035E-01	0.1316E 00	0.1164E 00	0.7112E-01	0.1236E-01	0.1015E-01	0.9959E-04	0.2257E-06	0.1313E-01	0.5542E-14
0.0150	0.6960E-02	0.1478E 00	0.9664E-01	0.5390E-01	0.9691E-02	0.8063E-02	0.1363E-03	0.3509E-06	0.1165E-01	0.9556E-14
0.0200	0.4365E-02	0.1583E 00	0.7367E-01	0.3734E-01	0.7327E-02	0.6250E-02	0.1877E-03	0.5585E-06	0.1029E-01	0.2151E-13
0.0231	0.3185E-02	0.1590E 00	0.5973E-01	0.2827E-01	0.6078E-02	0.5285E-02	0.2317E-03	0.7687E-06	0.9561E-02	0.1861E-13
0.0262	0.2223E-02	0.1551E 00	0.4649E-01	0.2025E-01	0.4954E-02	0.4409E-02	0.2863E-03	0.1065E-05	0.8929E-02	0.5113E-13
0.0294	0.1498E-02	0.1457E 00	0.3465E-01	0.1371E-01	0.3988E-02	0.3643E-02	0.3581E-03	0.1500E-05	0.8427E-02	0.6878E-13
0.0325	0.9597E-03	0.1310E 00	0.2443E-01	0.8614E-02	0.3159E-02	0.2973E-02	0.4503E-03	0.2140E-05	0.8060E-02	0.9792E-13
0.0356	0.5974E-03	0.1117E 00	0.1642E-01	0.5109E-02	0.2461E-02	0.2410E-02	0.5758E-03	0.3152E-05	0.7867E-02	0.1923E-12
0.0387	0.3486E-03	0.9013E-01	0.1027E-01	0.2744E-02	0.1916E-02	0.1927E-02	0.7433E-03	0.4702E-05	0.7834E-02	0.1350E-12
0.0450	0.1045E-03	0.4854E-01	0.3332E-02	0.6244E-03	0.1100E-02	0.1209E-02	0.1296E-02	0.1136E-04	0.8395E-02	0.8954E-12
0.0537	0.1424E-04	0.1351E-01	0.4484E-03	0.4427E-04	0.4734E-03	0.6120E-03	0.2594E-02	0.4428E-04	0.1054E-01	0.7310E-11
0.0625	0.1678E-05	0.2802E-02	0.4672E-04	0.2247E-05	0.1886E-03	0.3149E-03	0.6756E-02	0.1849E-03	0.1336E-01	0.5963E-10
0.0712	0.2018E-06	0.5328E-03	0.4710E-05	0.1113E-06	0.7030E-04	0.1643E-03	0.1374E-01	0.7622E-03	0.1477E-01	0.5181E-09
0.0800	0.2582E-07	0.1038E-03	0.5008E-06	0.5561E-08	0.2396E-04	0.9219E-04	0.2376E-01	0.2984E-02	0.1272E-01	0.3990E-08
0.0850	0.8414E-08	0.4198E-04	0.1467E-06	0.1146E-08	0.1254E-04	0.6681E-04	0.3000E-01	0.6138E-02	0.1037E-01	0.1182E-07
0.0925	0.1645E-08	0.1087E-04	0.2073E-07	0.4013E-10	0.4481E-05	0.4170E-04	0.3853E-01	0.1669E-01	0.6466E-02	0.5219E-07
0.1000	0.3387E-09	0.3208E-05	0.4402E-08	0.1134E-10	0.1493E-05	0.2624E-04	0.4505E-01	0.3940E-01	0.3384E-02	0.1753E-06
0.1100	0.4395E-10	0.6419E-06	0.4820E-09	0.6204E-12	0.3327E-06	0.1429E-04	0.5045E-01	0.8641E-01	0.1219E-02	0.4361E-06
0.1200	0.6250E-11	0.1345E-06	0.5740E-10	0.3787E-13	0.7680E-07	0.8059E-05	0.5442E-01	0.1241E 00	0.4373E-03	0.4656E-06
0.1300	0.8776E-12	0.3298E-07	0.8088E-11	0.2905E-14	0.2093E-07	0.4758E-05	0.5965E-01	0.1394E 00	0.1612E-03	0.4954E-06
0.1400	0.2217E-12	0.9035E-08	0.1437E-11	0.3030E-15	0.7084E-08	0.3061E-05	0.6793E-01	0.1473E 00	0.9685E-04	0.3527E-06
0.1500	0.5650E-13	0.2886E-08	0.3139E-12	0.3581E-16	0.2987E-08	0.2030E-05	0.8218E-01	0.1527E 00	0.6772E-04	0.2619E-06
0.1600	0.1675E-13	0.1055E-08	0.8147E-13	0.5948E-17	0.1534E-08	0.1363E-05	0.1057E 00	0.1577E 00	0.6143E-04	0.2084E-06
0.1700	0.5564E-14	0.4203E-09	0.2389E-13	0.1412E-17	0.9213E-09	0.9312E-06	0.1424E 00	0.1631E 00	0.6895E-04	0.1780E-06
0.1800	0.1972E-14	0.1755E-09	0.7514E-14	0.2394E-18	0.6092E-09	0.6518E-06	0.1949E 00	0.1692E 00	0.8653E-04	0.1619E-06
0.2000	0.2595E-15	0.2918E-10	0.7517E-15	0.1603E-19	0.2863E-09	0.3085E-06	0.3410E 00	0.1826E 00	0.1643E-03	0.1550E-06
0.2100	0.8844E-16	0.1067E-10	0.2164E-15	0.1708E-21	0.1867E-09	0.2105E-06	0.4221E 00	0.1891E 00	0.2138E-03	0.1581E-06
0.2200	0.2780E-16	0.3467E-11	0.5570E-16	0.1343E-21	0.1134E-09	0.1398E-06	0.4984E 00	0.1956E 00	0.2632E-03	0.1631E-06
0.2300	0.7837E-17	0.9926E-12	0.1243E-16	0.4653E-22	0.6352E-10	0.9158E-07	0.5640E 00	0.2006E 00	0.3057E-03	0.1686E-06
0.2400	0.1925E-17	0.2403E-12	0.2328E-17	0.2541E-21	0.3227E-10	0.5753E-07	0.6157E 00	0.2039E 00	0.3357E-03	0.1733E-06
0.2600	0.6826E-19	0.8143E-14	0.4191E-19	0.1238E-22	0.5908E-11	0.1956E-07	0.6765E 00	0.2087E 00	0.3488E-03	0.1770E-06
0.2800	0.2249E-20	0.1261E-15	0.1025E-20	0.1514E-22	0.6598E-12	0.4438E-08	0.6946E 00	0.2099E 00	0.3137E-03	0.1716E-06
0.3000	0.3758E-21	0.2001E-17	0.1027E-21	0.2436E-23	0.4059E-13	0.4017E-09	0.6922E 00	0.2089E 00	0.2605E-03	0.1588E-06
0.3300	0.2828E-22	0.7561E-21	0.2322E-21	0.6825E-22	0.1908E-15	0.3146E-11	0.6739E 00	0.2057E 00	0.1787E-03	0.1317E-06
0.3500	0.5545E-22	0.8713E-22	0.1573E-22	0.8828E-22	0.1763E-17	0.4725E-13	0.6582E 00	0.2031E 00	0.1376E-03	0.1150E-06
0.3800	0.3609E-22	0.6077E-21	0.1082E-21	0.7134E-21	0.4685E-18	0.2726E-13	0.6330E 00	0.1989E 00	0.9517E-04	0.9474E-07
0.4200	0.4609E-22	0.6984E-21	0.1007E-21	0.7351E-21	0.3220E-18	0.2128E-13	0.6018E 00	0.1938E 00	0.6326E-04	0.7625E-07
0.4400	0.5140E-22	0.7426E-21	0.9704E-22	0.7462E-21	0.2622E-18	0.2052E-13	0.5871E 00	0.1909E 00	0.5282E-04	0.6921E-07
0.4600	0.5869E-22	0.7971E-21	0.9467E-22	0.7577E-21	0.2066E-18	0.1747E-13	0.5709E 00	0.1880E 00	0.4369E-04	0.6245E-07
0.5000	0.6730E-22	0.8511E-21	0.9231E-22	0.7633E-21	0.1788E-18	0.1624E-13	0.5546E 00	0.1850E 00	0.3626E-04	0.5645E-07
0.5400	0.7841E-22	0.9201E-21	0.9099E-22	0.7621E-21	0.1278E-18	0.2618E-13	0.5371E 00	0.1816E 00	0.2989E-04	0.5075E-07
0.5600	0.8359E-22	0.9487E-21	0.9006E-22	0.7883E-21	0.1126E-18	0.2606E-13	0.5294E 00	0.1801E 00	0.2750E-04	0.4847E-07
0.5800	0.8885E-22	0.9765E-21	0.8908E-22	0.7939E-21	0.7916E-19	0.2526E-13	0.5220E 00	0.1786E 00	0.2538E-04	0.4636E-07
0.6200	0.1000E-21	0.1025E-20	0.8626E-22	0.7995E-21	0.7061E-19	0.2388E-13	0.5063E 00	0.1755E 00	0.2148E-04	0.4225E-07
0.6400	0.1000E-21	0.1025E-20	0.8626E-22	0.7995E-21	0.7061E-19	0.2388E-13	0.5063E 00	0.1755E 00	0.2148E-04	0.4225E-07
0.6800	0.1129E-21	0.1075E-20	0.8392E-22	0.8111E-21	0.5990E-19	0.2177E-13	0.4912E 00	0.1724E 00	0.1632E-04	0.3864E-07
0.7000	0.1260E-21	0.1123E-20	0.8169E-22	0.8223E-21	0.2768E-19	0.4318E-14	0.4774E 00	0.1695E 00	0.1585E-04	0.3560E-07
0.7400	0.1407E-21	0.1179E-20	0.7914E-22	0.8327E-21	0.1804E-19	0.5661E-14	0.4631E 00	0.1664E 00	0.1366E-04	0.3272E-07
0.7600	0.1407E-21	0.1179E-20	0.7914E-22	0.8327E-21	0.1804E-19	0.5661E-14	0.4631E 00	0.1664E 00	0.1366E-04	0.3272E-07
0.8000	0.1572E-21	0.1231E-20	0.7643E-22	0.8433E-21	0.1243E-19	0.7732E-14	0.4487E 00	0.1633E 00	0.1176E-04	0.3002E-07
0.8200	0.1757E-21	0.1283E-20	0.7358E-22	0.8542E-21	0.8626E-20	0.7627E-14	0.4342E 00	0.1600E 00	0.1011E-04	0.2751E-07
0.8600	0.6098E-21	0.2401E-20	0.2228E-21	0.2567E-22	0.7633E-20	0.1765E-13	0.4190E 00	0.1564E 00	0.8621E-05	0.2507E-07
0.8800	0.6098E-21	0.2401E-20	0.2227E-21	0.2570E-22	0.7633E-20	0.1765E-13	0.4190E 00	0.1564E 00	0.8621E-05	0.2507E-07
0.9200	0.7002E-21	0.2500E-20	0.2157E-21	0.2604E-22	0.6860E-20	0.1678E-13	0.4029E 00	0.1526E 00	0.7274E-05	0.2269E-07
0.9400	0.8064E-21	0.2618E-20	0.2079E-21	0.2640E-22	0.6044E-20	0.1585E-13	0.3865E 00	0.1486E 00	0.6110E-05	0.2045E-07
0.9800	0.3886E-22	0.4124E-21	0.2066E-21	0.2696E-22	0.9429E-21	0.1486E-13	0.3674E 00	0.1438E 00	0.4971E-05	0.1795E-07
1.0000	0.4440E-22	0.4394E-21	0.2040E-21	0.2721E-22	0.1004E-20	0.1295E-13	0.3546E 00	0.1404E 00	0.4314E-05	0.1638E-07

EQUILIBRIUM MOLE FRACTIONS

ETA	C+	H	N+	O+	E-	C	CN	CO	C2	C2H
0.0	0.5703E-04	0.5106E 00	0.1025E-10	0.5351E-13	0.2531E-10	0.1485E-01	0.2153E-01	0.1145E 00	0.1424E-01	0.3458E-01
0.0050	0.5478E-05	0.5384E 00	0.3852E-11	0.4697E-14	0.1759E-09	0.2147E-01	0.2334E-01	0.1100E 00	0.1926E-01	0.9029E-01
0.0100	-0.4730E-11	0.5612E 00	-0.3248E-17	-0.4152E-20	0.5681E-07	0.3134E-01	0.2485E-01	0.1055E 00	0.258[illegible]E-01	0.9134E-01
0.0150	0.4403E-08	0.5794E 00	0.9763E-15	0.4017E-17	0.5745E-12	0.4479E-01	0.2599E-01	0.1009E 00	0.3363E-01	0.7425E-01
0.0200	0.1602E-06	0.5925E 00	0.3591E-13	0.4268E-15	0.1639E-10	0.6325E-01	0.2670E-01	0.9630E-01	0.4250E-01	0.6295E-01
0.0231	0.4796E-08	0.5975E 00	0.2908E-14	0.1300E-16	0.1719E-12	0.7830E-01	0.2686E-01	0.9339E-01	0.4818E-01	0.5504E-01
0.0262	0.1990E-06	0.6004E 00	0.1110E-12	0.8866E-15	-0.1589E-11	0.9574E-01	0.2684E-01	0.9051E-01	0.5151E-01	0.4683E-01
0.0294	0.4793E-09	0.6008E 00	0.2441E-15	0.1501E-17	0.1298E-07	0.1159E 00	0.2664E-01	0.8769E-01	0.5800E-01	0.3864E-01
0.0325	0.6750E-13	0.5991E 00	0.3760E-19	0.3665E-21	0.4987E-05	0.1384E 00	0.2628E-01	0.8496E-01	0.6124E-01	0.3077E-01
0.0356	0.2070E-09	0.5951E 00	0.1537E-15	0.3363E-17	0.3108E-05	0.1634E 00	0.2575E-01	0.8239E-01	0.6250E-01	0.2361E-01
0.0387	-0.6413E-13	0.5893E 00	-0.8169E-19	-0.9575E-21	0.5957E-03	0.1895E 00	0.2508E-01	0.7994E-01	0.6166E-01	0.1734E-01
0.0450	0.1620E-06	0.5759E 00	0.2056E-12	0.3345E-14	0.4839E-03	0.2422E 00	0.2341E-01	0.7591E-01	0.5337E-01	0.8240E-02
0.0537	0.1136E-05	0.5585E 00	0.4277E-11	0.4989E-13	0.4622E-03	0.3023E 00	0.2028E-01	0.7214E-01	0.3392E-01	0.2231E-02
0.0625	0.6662E-05	0.5472E 00	0.4558E-10	0.1774E-11	0.4590E-03	0.3385E 00	0.1623E-01	0.7010E-01	0.1776E-01	0.5157E-03
0.0712	0.1310E-03	0.5400E 00	0.5021E-08	0.2981E-09	0.1222E-03	0.3578E 00	0.1179E-01	0.6890E-01	0.8659E-02	0.1170E-03
0.0800	0.2825E-03	0.5346E 00	0.2683E-07	0.3182E-08	0.2599E-03	0.3682E 00	0.7571E-02	0.6718E-01	0.4188E-02	0.2740E-04
0.0850	0.4230E-03	0.5316E 00	0.6196E-07	0.1127E-07	0.3943E-03	0.3721E 00	0.5580E-02	0.6539E-01	0.2603E-02	0.1239E-04
0.0925	0.7643E-03	0.5262E 00	0.1919E-06	0.6766E-07	0.7189E-03	0.3777E 00	0.3282E-02	0.6001E-01	0.1562E-02	0.3496E-05
0.1000	0.1362E-02	0.5186E 00	0.5259E-06	0.3447E-06	0.1300E-02	0.3850E 00	0.1788E-02	0.4902E-01	0.6920E-03	0.1270E-05
0.1100	0.2905E-02	0.5052E 00	0.1766E-05	0.2037E-05	0.2798E-02	0.3966E 00	0.7470E-03	0.2725E-01	0.4365E-03	0.2988E-06
0.1200	0.5919E-02	0.4936E 00	0.5442E-05	0.7571E-05	0.5734E-02	0.4022E 00	0.3148E-03	0.1061E-01	0.2164E-03	0.7435E-07
0.1300	0.9571E-02	0.4863E 00	0.1340E-04	0.2057E-04	0.9242E-02	0.4005E 00	0.5994E-04	0.4332E-02	0.1110E-03	0.2082E-07
0.1400	0.1616E-01	0.4771E 00	0.3476E-04	0.4616E-04	0.1578E-01	0.3918E 00	0.3453E-04	0.1670E-02	0.6121E-04	0.[illegible]795E-08
0.1500	0.2499E-01	0.4633E 00	0.8546E-04	0.9185E-04	0.2446E-01	0.3787E 00	0.2340E-04	0.7374E-03	0.3600E-04	0.2543E-08
0.1600	0.3573E-01	0.4432E 00	0.2027E-03	0.1672E-03	0.3470E-01	0.3618E 00	0.1853E-04	0.3741E-03	0.2242E-04	0.1[illegible]E-08
0.1700	0.4715E-01	0.4180E 00	0.4609E-03	0.2817E-03	0.4572E-01	0.3392E 00	0.1654E-04	0.2134E-03	0.1440E-04	0.4863E-09
0.1800	0.5754E-01	0.3888E 00	0.9908E-03	0.4466E-03	0.5655E-01	0.3096E 00	0.1584E-04	0.1333E-03	0.9335E-05	0.2326E-09
0.2000	0.6868E-01	0.3224E 00	0.3660E-02	0.9802E-03	0.7317E-01	0.2311E 00	0.1471E-04	0.6169E-04	0.3605E-05	0.5323E-10
0.2100	0.6794E-01	0.2872E 00	0.6289E-02	0.1391E-02	0.7798E-01	0.1862E 00	0.1323E-04	0.4294E-04	0.2045E-05	0.2388E-10
0.2200	0.6291E-01	0.2519E 00	0.1009E-01	0.1928E-02	0.8025E-01	0.1422E 00	0.1106E-04	0.2940E-04	0.1068E-05	0.9852E-11
0.2300	0.5451E-01	0.2168E 00	0.1525E-01	0.2617E-02	0.8059E-01	0.1023E 00	0.8528E-05	0.1944E-04	0.5036E-06	0.3665E-11
0.2400	0.4391E-01	0.1825E 00	0.2184E-01	0.3476E-02	0.7968E-01	0.6909E-01	0.6009E-05	0.1220E-04	0.2113E-06	0.1200E-11
0.2600	0.2238E-01	0.1175E 00	0.3870E-01	0.5660E-02	0.7614E-01	0.2572E-01	0.2260E-05	0.3926E-05	0.253[illegible]E-07	0.[illegible]071E-13
0.2800	0.8291E-02	0.6081E-01	0.5702E-01	0.8078E-02	0.8116E-01	0.7554E-02	0.6182E-06	0.9751E-06	0.150[illegible]	0.2794E-14
0.3000	0.2603E-02	0.1951E-01	0.7334E-01	0.1027E-01	0.6590E-01	0.2025E-02	0.1464E-06	0.2141E-06	0.1205E-[illegible]	0.2949E-16
0.3300	0.2672E-03	0.1851E-02	0.9429E-01	0.1315E-01	0.1096E 00	0.1719E-03	0.9563E-08	0.1269E-07	0.7175E-12	0.2441E-1[illegible]
0.3500	0.3550E-04	0.2354E-03	0.1075E 00	0.1504E-01	0.1243E 00	0.2037E-04	0.9437E-09	0.1164E-08	0.693[illegible]E-14	0.2044E-21
0.3800	0.3701E-04	0.2297E-03	0.1269E 00	0.1787E-01	0.1466E 00	0.1818E-04	0.6073E-09	0.7130E-09	0.5[illegible]E-14	0.1020E-20
0.4200	0.3834E-04	0.2230E-03	0.1495E 00	0.2133E-01	0.1728E 00	0.1589E-04	0.3284E-09	0.3637E-09	0.2616E-14	0.13[illegible]E-20
0.4400	0.3886E-04	0.2200E-03	0.1598E 00	0.2295E-01	0.1647E 00	0.1496E-04	0.2359E-09	0.2550E-09	0.152[illegible]E-14	0.14[illegible]E-20
0.4800	0.3934E-04	0.2167E-03	0.1706E 00	0.2472E-01	0.1573E 00	0.1403E-04	0.1552E-09	0.1636E-09	0.5[illegible]	0.1552E-20
0.5000	0.3962E-04	0.2135E-03	0.1812E 00	0.2649E-01	0.2097E 00	0.1311E-04	0.1073E-09	0.1097E-09	0.6111E-16	0.1610E-20
0.5400	0.3998E-04	0.2101E-03	0.1923E 00	0.2840E-01	0.2227E 00	0.1226E-04	0.1935E-10	0.1850E-10	0.485[illegible]E-16	0.43[illegible]E-22
0.5600	0.4014E-04	0.2087E-03	0.1970E 00	0.2924E-01	0.2283E 00	0.1191E-04	0.1012E-10	0.8503E-11	0.3171E-1[illegible]	0.5037E-22
0.5800	0.4030E-04	0.2073E-03	0.2015E 00	0.3005E-01	0.2336E 00	0.1156E-04	0.9762E-11	0.7459E-11	0.6141E-15	0.5076E-22
0.6200	0.4043E-04	0.2045E-03	0.2108E 00	0.3175E-01	0.2446E 00	0.1089E-04	0.3386E-10	0.2384E-10	0.12[illegible]E-14	0.5092E-22
0.6400	0.4043E-04	0.2045E-03	0.2108E 00	0.3175E-01	0.2446E 00	0.1089E-04	0.3386E-10	0.2384E-10	0.1235E-14	0.5092E-22
0.6800	0.4054E-04	0.2017E-03	0.2195E 00	0.3340E-01	0.2549E 00	0.1027E-04	0.3074E-10	0.1872E-10	0.1065E-14	0.5095E-22
0.7000	0.4063E-04	0.1953E-03	0.2272E 00	0.3491E-01	0.2642E 00	0.9735E-05	0.9450E-10	0.8698E-10	0.9077E-15	0.5409E-22
0.7400	0.4070E-04	0.1969E-03	0.2350E 00	0.3647E-01	0.2735E 00	0.9218E-05	0.8644E-10	0.8026E-10	0.7270E-15	0.5766E-22
0.7600	0.4070E-04	0.1969E-03	0.2350E 00	0.3647E-01	0.2735E 00	0.9218E-05	0.8644E-10	0.8026E-10	0.7270E-15	0.5766E-22
0.8000	0.4075E-04	0.1945E-03	0.2426E 00	0.3806E-01	0.2827E 00	0.8722E-05	0.6620E-10	0.6087E-10	0.5737E-15	0.6138E-22
0.8200	0.4078E-04	0.1921E-03	0.2501E 00	0.3967E-01	0.2918E 00	0.8250E-05	0.4210E-10	0.3833E-10	0.3704E-15	0.6523E-22
0.8600	0.4079E-04	0.1897E-03	0.2578E 00	0.4137E-01	0.3011E 00	0.7778E-05	0.2814E-10	0.2340E-10	0.6752E-16	0.1358E-21
0.8800	0.4079E-04	0.1897E-03	0.2578E 00	0.4137E-01	0.3011E 00	0.7778E-05	0.2814E-10	0.2340E-10	0.6753E-16	0.1358E-21
0.9200	0.4078E-04	0.1871E-03	0.2656E 00	0.4319E-01	0.3108E 00	0.7305E-05	0.2897E-10	0.2422E-10	0.6367E-16	0.1519E-21
0.9400	0.4075E-04	0.1846E-03	0.2734E 00	0.4504E-01	0.3203E 00	0.6850E-05	0.2779E-10	0.2326E-10	0.5949E-16	0.166[illegible]E-21
0.9800	0.4084E-04	0.1818E-03	0.2821E 00	0.4723E-01	0.3312E 00	0.6372E-05	0.3108E-10	0.2742E-10	0.2521E-15	0.7735E-21
1.0000	0.4084E-04	0.1800E-03	0.2878E 00	0.4872E-01	0.3384E 00	0.6056E-05	0.2178E-10	0.1934E-10	0.1777E-15	0.6325E-21

EQUILIBRIUM MOLE FRACTIONS

ETA	C2H2	C3	C3H	C4H	HCN	H2	N	O	N2	O2
0.0	0.9537E-02	0.3253E-01	0.5206E-01	0.2641E-01	0.8516E-02	0.9326E-01	0.4669E-04	0.7552E-07	0.7155E-02	0.1306E-14
0.0050	0.6687E-02	0.3745E-01	0.4457E-01	0.2147E-01	0.6764E-02	0.7399E-01	0.6157E-04	0.1088E-06	0.6247E-02	0.2036E-14
0.0100	0.4552E-02	0.4185E-01	0.3661E-01	0.1661E-01	0.5241E-02	0.5766E-01	0.8145E-04	0.1416E-06	0.5370E-02	0.1984E-14
0.0150	0.2930E-02	0.4498E-01	0.2820E-01	0.1205E-01	0.3931E-02	0.4388E-01	0.1067E-03	0.2404E-06	0.4560E-02	0.3274E-14
0.0200	0.1754E-02	0.4595E-01	0.2081E-01	0.7963E-02	0.2836E-02	0.3243E-01	0.1402E-03	0.3651E-06	0.3841E-02	0.7031E-14
0.0231	0.1241E-02	0.4477E-01	0.1636E-01	0.5846E-02	0.2282E-02	0.2660E-01	0.1678E-03	0.4875E-06	0.3463E-02	0.5900E-14
0.0262	0.8395E-03	0.4233E-01	0.1234E-01	0.4059E-02	0.1802E-02	0.2150E-01	0.2014E-03	0.6543E-06	0.3134E-02	0.1571E-13
0.0294	0.5481E-03	0.3851E-01	0.8912E-02	0.2663E-02	0.1406E-02	0.1722E-01	0.2435E-03	0.8931E-06	0.2865E-02	0.2048E-13
0.0325	0.3402E-03	0.3356E-01	0.6088E-02	0.1621E-02	0.1079E-02	0.1361E-01	0.2967E-03	0.1234E-05	0.2655E-02	0.2824E-13
0.0356	0.2053E-03	0.2775E-01	0.3966E-02	0.9320E-03	0.8217E-03	0.1070E-01	0.3679E-03	0.1763E-05	0.2513E-02	0.5377E-13
0.0387	0.1163E-03	0.2172E-01	0.2407E-02	0.4256E-03	0.6155E-03	0.8301E-02	0.4608E-03	0.2552E-05	0.2430E-02	0.3663E-13
0.0450	0.3310E-04	0.1111E-01	0.7416E-03	0.1050E-03	0.3374E-03	0.4947E-02	0.7631E-03	0.5855E-05	0.2471E-02	0.2307E-12
0.0537	0.4285E-05	0.2936E-02	0.9488E-04	0.7073E-05	0.1373E-03	0.2379E-02	0.1675E-02	0.2169E-04	0.2950E-02	0.1790E-11
0.0625	0.4914E-06	0.5928E-03	0.5614E-05	0.3492E-06	0.5320E-04	0.1191E-02	0.3676E-02	0.8611E-04	0.3635E-02	0.1421E-10
0.0712	0.5825E-07	0.1112E-03	0.9558E-06	0.1706E-07	0.1555E-04	0.6151E-03	0.7374E-02	0.3581E-03	0.3964E-02	0.1217E-09
0.0800	0.7377E-08	0.2136E-04	0.1006E-06	0.8435E-09	0.6600E-05	0.3402E-03	0.1262E-01	0.1387E-02	0.3378E-02	0.9275E-09
0.0850	0.2391E-08	0.8622E-05	0.2931E-07	0.1730E-09	0.3434E-05	0.2453E-03	0.1585E-01	0.2839E-02	0.2739E-02	0.2734E-08
0.0925	0.4634E-09	0.2212E-05	0.4104E-08	0.6009E-11	0.1216E-05	0.1517E-03	0.2020E-01	0.7649E-02	0.1693E-02	0.1196E-07
0.1000	0.9420E-10	0.6446E-06	0.8604E-09	0.1674E-11	0.4017E-06	0.9426E-04	0.2329E-01	0.1783E-01	0.8745E-03	0.3967E-07
0.1100	0.1195E-10	0.1261E-06	0.9210E-10	0.8953E-13	0.8714E-07	0.5018E-04	0.2549E-01	0.3822E-01	0.3081E-03	0.9645E-07
0.1200	0.1670E-11	0.2596E-07	0.1078E-10	0.5370E-14	0.1577E-07	0.2781E-04	0.2702E-01	0.5395E-01	0.1086E-03	0.1035E-06
0.1300	0.2332E-12	0.6334E-08	0.1511E-11	0.4098E-15	0.5359E-08	0.1633E-04	0.2947E-01	0.6029E-01	0.4476E-04	0.1071E-06
0.1400	0.5893E-13	0.1736E-08	0.2685E-12	0.4276E-16	0.1814E-08	0.1051E-04	0.3357E-01	0.6374E-01	0.2393E-04	0.7630E-07
0.1500	0.1514E-13	0.5550E-09	0.5915E-13	0.5096E-17	0.7715E-09	0.7029E-05	0.4095E-01	0.6660E-01	0.1687E-04	0.5711E-07
0.1600	0.4575E-14	0.2083E-09	0.1564E-13	0.6626E-18	0.4037E-09	0.4808E-05	0.5369E-01	0.7009E-01	0.1560E-04	0.4633E-07
0.1700	0.1563E-14	0.8531E-10	0.4717E-14	0.2105E-18	0.2495E-09	0.3379E-05	0.7437E-01	0.7455E-01	0.1800E-04	0.4068E-07
0.1800	0.5751E-15	0.3697E-10	0.1540E-14	0.3705E-19	0.1711E-09	0.2455E-05	0.1056E 00	0.8026E-01	0.2400E-04	0.3841E-07
0.2000	0.8360E-16	0.6792E-11	0.1702E-15	0.2742E-20	0.8503E-10	0.1283E-05	0.2042E 00	0.9571E-01	0.4918E-04	0.4062E-07
0.2100	0.3019E-16	0.2632E-11	0.5194E-16	0.3094E-22	0.6138E-10	0.9279E-06	0.2678E 00	0.1050E 00	0.6782E-04	0.4391E-07
0.2200	0.1007E-16	0.9131E-12	0.1419E-16	0.2582E-22	0.3559E-10	0.6541E-06	0.3357E 00	0.1150E 00	0.8864E-04	0.4808E-07
0.2300	0.3011E-17	0.2756E-12	0.3356E-17	0.9489E-23	0.2351E-10	0.4544E-06	0.4027E 00	0.1250E 00	0.1092E-03	0.5270E-07
0.2400	0.7814E-18	0.7051E-13	0.6643E-18	0.5476E-22	0.1262E-10	0.3016E-06	0.4646E 00	0.1347E 00	0.1267E-03	0.5725E-07
0.2600	0.3042E-19	0.2623E-14	0.1313E-19	0.2928E-23	0.2537E-11	0.1126E-06	0.5604E 00	0.1513E 00	0.1445E-03	0.6418E-07
0.2800	0.1070E-20	0.4335E-16	0.3427E-21	0.3825E-23	0.3025E-12	0.2726E-07	0.6144E 00	0.1625E 00	0.1387E-03	0.6645E-07
0.3000	0.1853E-21	0.7131E-18	0.3560E-22	0.6377E-24	0.1529E-13	0.2559E-08	0.6346E 00	0.1676E 00	0.1194E-03	0.6372E-07
0.3300	0.1390E-22	0.2687E-21	0.8025E-22	0.2303E-22	0.9039E-16	0.1998E-10	0.6159E 00	0.1646E 00	0.8166E-04	0.5268E-07
0.3500	0.2686E-22	0.3050E-22	0.5356E-23	0.2270E-22	0.6227E-18	0.2956E-12	0.5926E 00	0.1601E 00	0.6153E-04	0.4532E-07
0.3800	0.1704E-22	0.2073E-21	0.3591E-22	0.1788E-21	0.2131E-18	0.1663E-12	0.5555E 00	0.1528E 00	0.4175E-04	0.3639E-07
0.4200	0.2109E-22	0.2309E-21	0.3238E-22	0.1786E-21	0.1419E-18	0.1256E-12	0.5119E 00	0.1441E 00	0.2690E-04	0.2839E-07
0.4400	0.2318E-22	0.2418E-21	0.3076E-22	0.1787E-21	0.1139E-18	0.1195E-12	0.4921E 00	0.1401E 00	0.2214E-04	0.2540E-07
0.4800	0.2606E-22	0.2557E-21	0.2955E-22	0.1786E-21	0.8839E-19	0.1002E-12	0.4712E 00	0.1358E 00	0.1803E-04	0.2256E-07
0.5000	0.2942E-22	0.2689E-21	0.2837E-22	0.1771E-21	0.7532E-19	0.9166E-13	0.4507E 00	0.1316E 00	0.1473E-04	0.2008E-07
0.5400	0.3371E-22	0.2859E-21	0.2750E-22	0.1785E-21	0.5295E-19	0.1454E-12	0.4292E 00	0.1271E 00	0.1195E-04	0.1776E-07
0.5600	0.3568E-22	0.2927E-21	0.2702E-22	0.1786E-21	0.4629E-19	0.1437E-12	0.4201E 00	0.1251E 00	0.1091E-04	0.1684E-07
0.5800	0.3766E-22	0.2951E-21	0.2655E-22	0.1787E-21	0.3233E-19	0.1383E-12	0.4113E 00	0.1232E 00	0.9993E-05	0.1599E-07
0.6200	0.4179E-22	0.3095E-21	0.2534E-22	0.1773E-21	0.2843E-19	0.1289E-12	0.3933E 00	0.1193E 00	0.8343E-05	0.1437E-07
0.6400	0.4179E-22	0.3095E-21	0.2534E-22	0.1773E-21	0.2843E-19	0.1289E-12	0.3933E 00	0.1193E 00	0.8343E-05	0.1437E-07
0.6800	0.4653E-22	0.3213E-21	0.2431E-22	0.1774E-21	0.2378E-19	0.1159E-12	0.3763E 00	0.1156E 00	0.7016E-05	0.1296E-07
0.7000	0.5129E-22	0.3320E-21	0.2337E-22	0.1777E-21	0.1086E-19	0.2270E-13	0.3612E 00	0.1123E 00	0.5995E-05	0.1179E-07
0.7400	0.5655E-22	0.3424E-21	0.2236E-22	0.1776E-21	0.6985E-20	0.2938E-13	0.3460E 00	0.1089E 00	0.5103E-05	0.1070E-07
0.7600	0.5655E-22	0.3424E-21	0.2236E-22	0.1776E-21	0.6985E-20	0.2938E-13	0.3460E 00	0.1089E 00	0.5103E-05	0.1070E-07
0.8000	0.6239E-22	0.3529E-21	0.2132E-22	0.1776E-21	0.4750E-20	0.3963E-13	0.3310E 00	0.1054E 00	0.4336E-05	0.9694E-08
0.8200	0.6884E-22	0.3633E-21	0.2026E-22	0.1776E-21	0.3256E-20	0.3859E-13	0.3162E 00	0.1020E 00	0.3681E-05	0.8769E-08
0.8600	0.2357E-21	0.6707E-21	0.6053E-22	0.5269E-23	0.2843E-20	0.8812E-13	0.3011E 00	0.9843E-01	0.3098E-05	0.7888E-08
0.8800	0.2357E-21	0.6707E-21	0.6053E-22	0.5274E-23	0.2843E-20	0.8812E-13	0.3011E 00	0.9843E-01	0.3098E-05	0.7888E-08
0.9200	0.2670E-21	0.6904E-21	0.5780E-22	0.5270E-23	0.2520E-20	0.8262E-13	0.2855E 00	0.9468E-01	0.2577E-05	0.7039E-08
0.9400	0.3032E-21	0.7113E-21	0.5494E-22	0.5265E-23	0.2169E-20	0.7697E-13	0.2701E 00	0.9091E-01	0.2135E-05	0.6255E-08
0.9800	0.1438E-22	0.1102E-21	0.5373E-22	0.5299E-23	0.3306E-21	0.7099E-13	0.2526E 00	0.8655E-01	0.1709E-05	0.5403E-08
1.0000	0.1625E-22	0.1162E-21	0.5249E-22	0.5286E-23	0.3540E-21	0.6121E-13	0.2412E 00	0.8362E-01	0.1467E-05	0.4876E-08

APPENDIX H

GRAPHICAL RESULTS OF CASES RUN

In Table 6.2. a tabular summary of the results of this study is given. This appendix includes figures corresponding to the summarized results of Table 6.2. Figures H-1 through H-8 present the temperature, velocity, velocity function, and radiative flux divergence for each case examined.

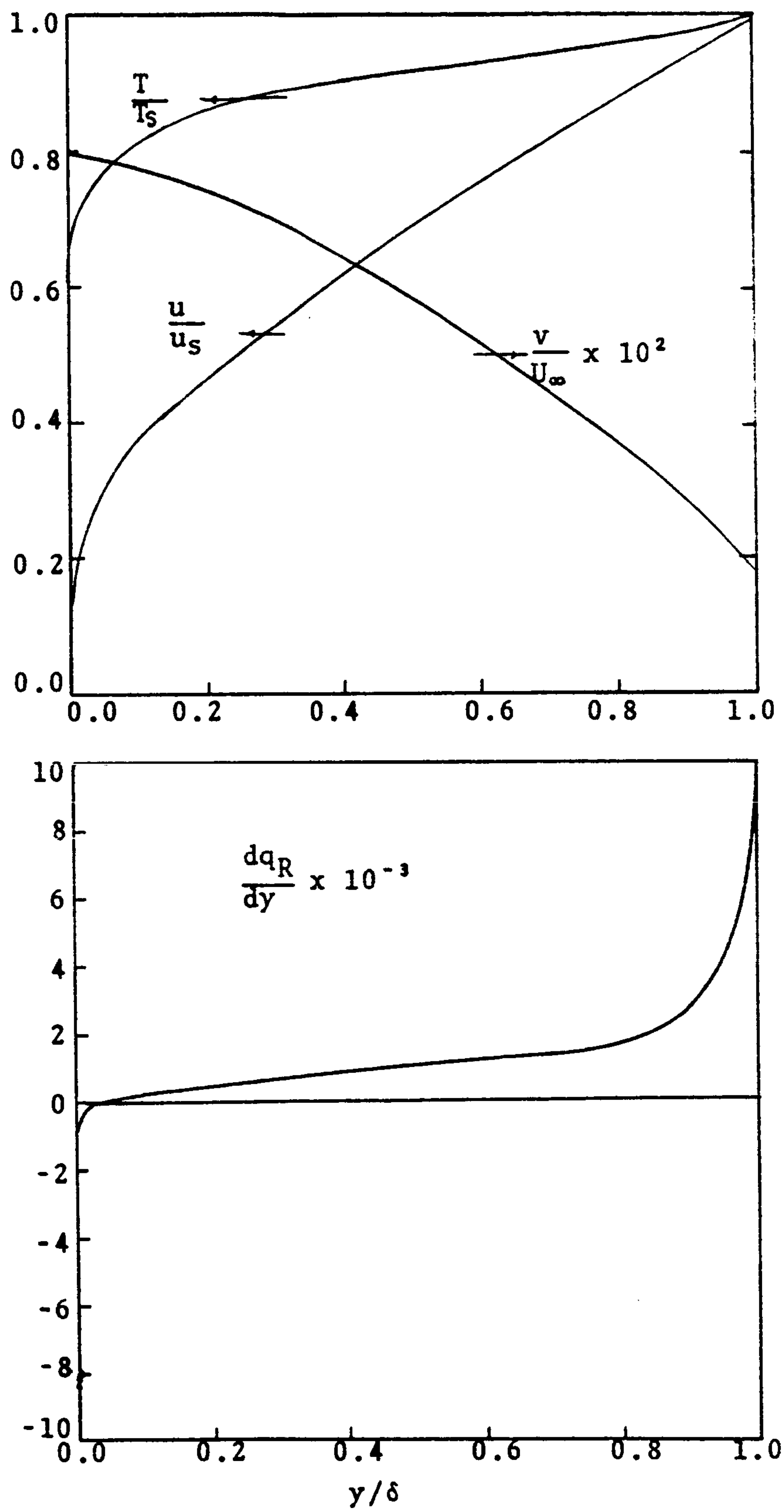


Figure H-1. Case Number 1.

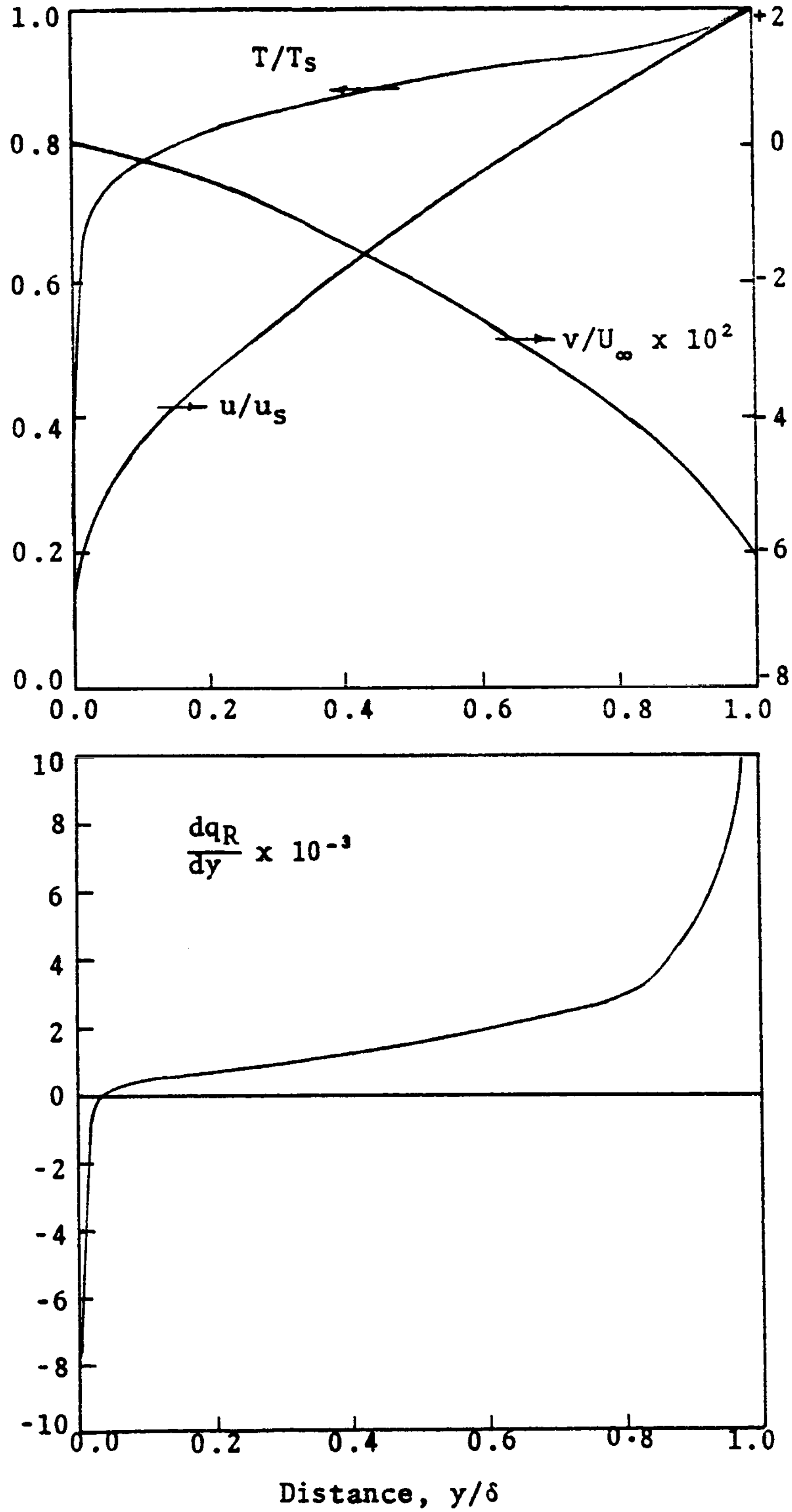


Figure H-2. Case Number 2.

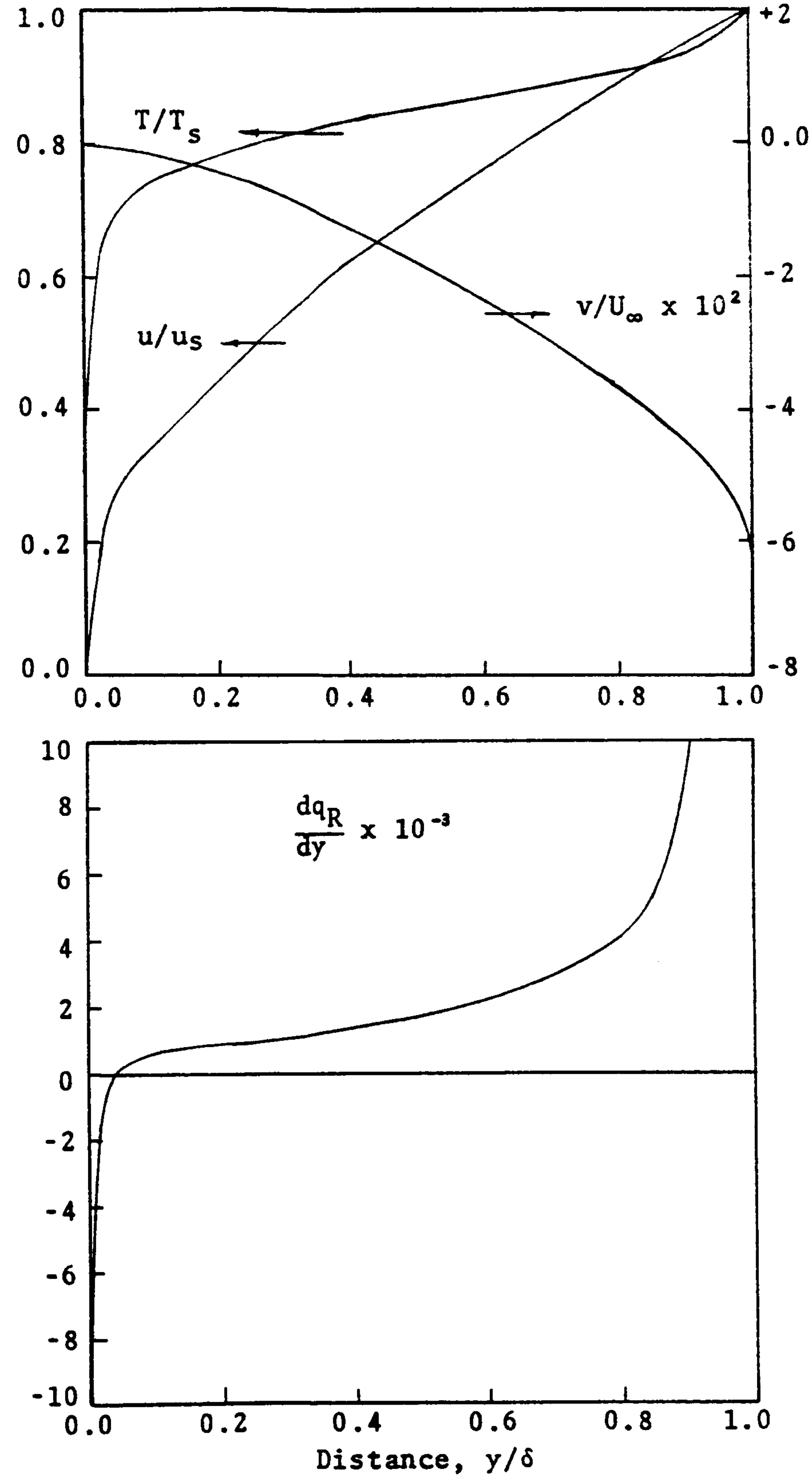


Figure H-3. Case Number 3.

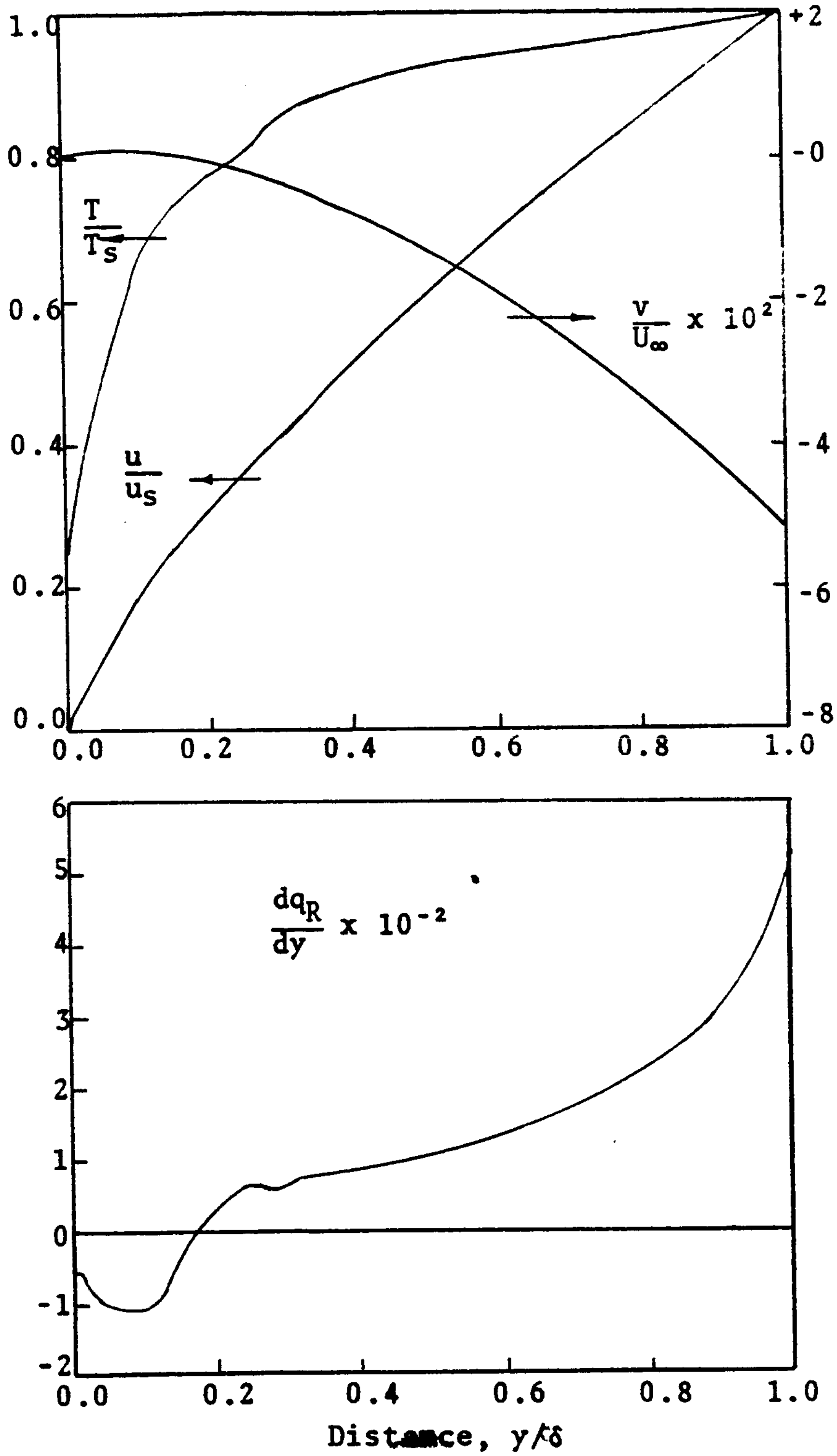


Figure H-4. Cases 4 and 5.

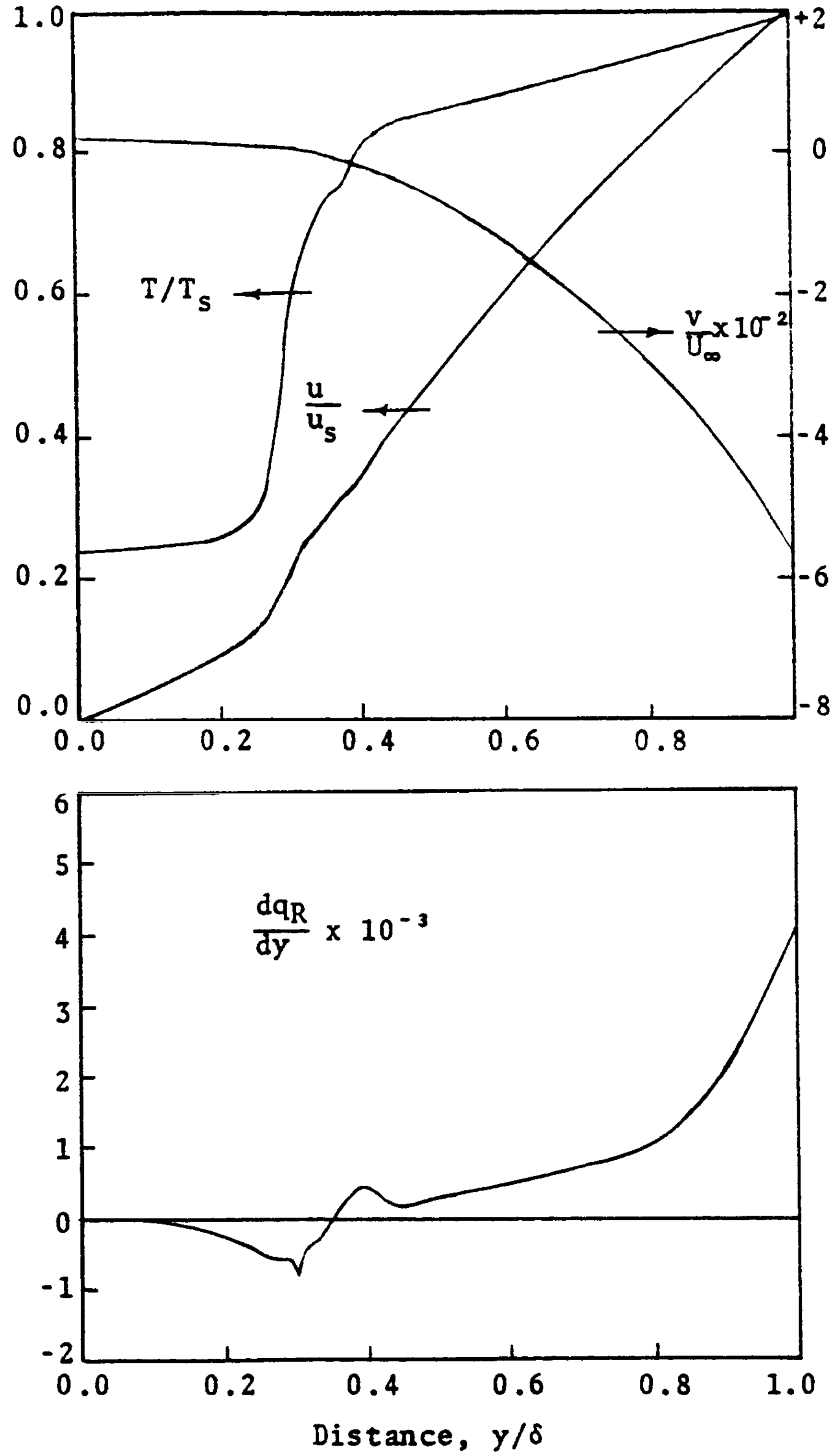


Figure H-5. Cases 6 and 7.

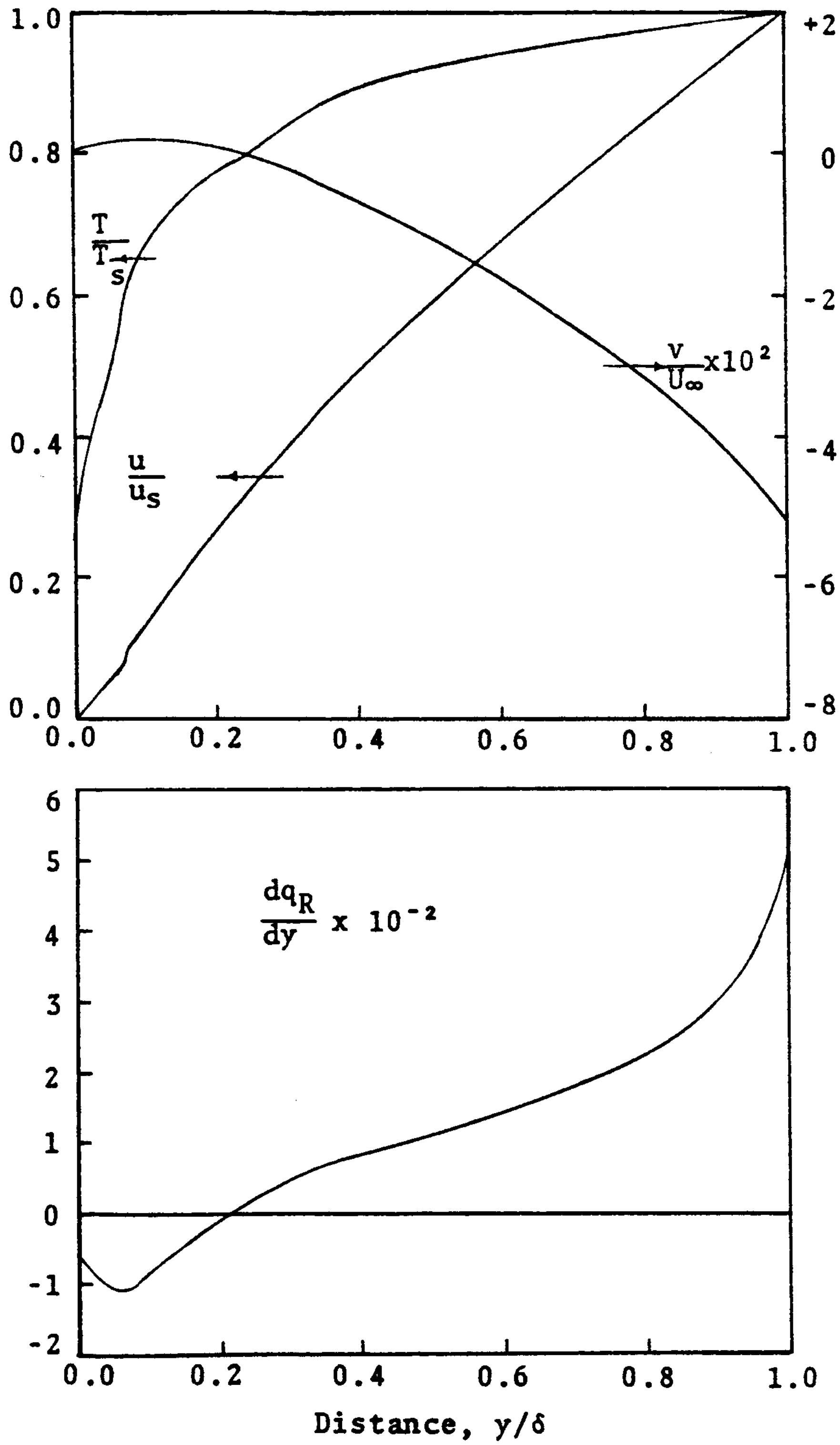
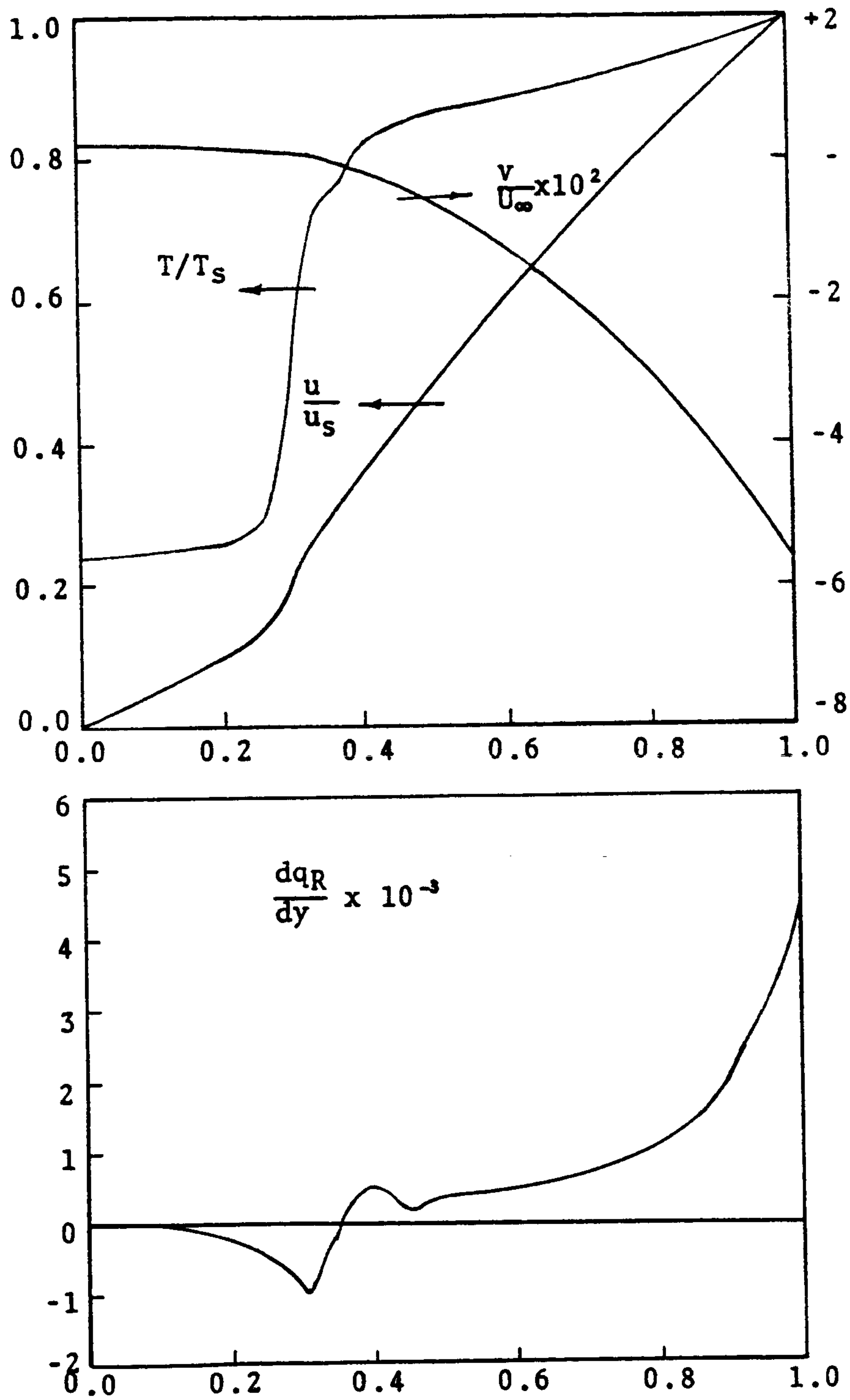


Figure H-6. Case Number 8.



Distance, y/δ

Figure H-7. Case Number 9.

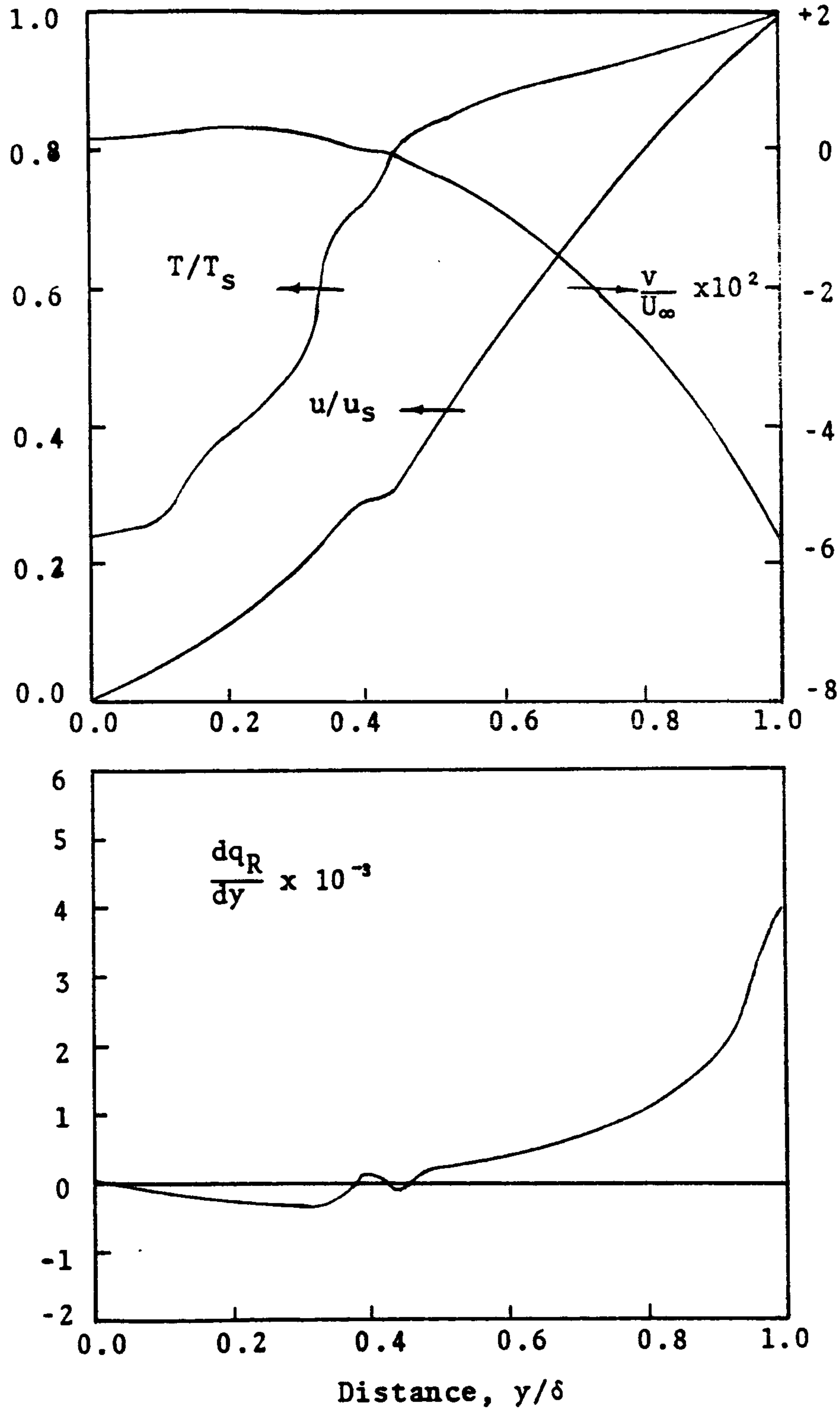


Figure H-8. Case Number 10.

APPENDIX I

POSTERIORI EXAMINATION OF SORET EFFECT

A conservative estimate of the maximum thermal diffusion effect that could be expected from the results of this study is given in this appendix. The examination proceeds as follows:

The contribution of temperature gradients toward mass diffusion is given by the following equation (from Eq. 2.1),

$$J_i = D_i^T \frac{d\ln T}{dy} \tag{I-1}$$

From Reference I-1, a large value of the binary thermal diffusion ratio $(M^2 D_A^T/\rho M_A M_B D_{AB})$ is seen to be on the order of 10^{-1}. Assuming that the molecular weights are of equal orders of magnitude,

$$\frac{D_A^T}{\rho \mathcal{D}_{AB}} \approx 10^{-1} \tag{I-2}$$

The most severe temperature gradient encountered in this study appeared in Case 6 (Figure H-5) at $y/\delta \approx 0.28$. The gradient in the log of the temperature at that point was computed to be $36.2^{\circ}K/ft$. At the same point, a liberal estimate of the binary diffusion coefficient ($\mathcal{D}_{AB}$) is 4.0 x 10^{-} (D_{H-H}). From these estimates, and the corresponding value of the density, the non-dimensional mass flux ($J_i/\rho_s U_\infty$) was computed as ≈ 0.5 x 10^{-5}. In Table I-1, a tabulation of the predicted (multicomponent) mass fluxes is given for the same point of analysis. From these values, it is clearly shown that the maximum estimated mass flux due to thermal diffusion is at least an order of magnitude less than the significant species fluxes due to concentration differences.

TABLE I-1

MASS FLUXES OF PRINCIPLE SPECIES FOR CASE NUMBER SIX AT $y/\delta = 0.28$

Species	Mass Flux $J_i/\rho_s U_\infty$
H_2	0.3756×10^{-6}
N	-0.1555×10^{-4}
O	-0.4416×10^{-4}
N_2	0.1110×10^{-4}
C^+	-0.1118×10^{-5}
H	0.1014×10^{-4}
C	-0.1568×10^{-3}
CN	0.2543×10^{-4}
CO	0.1562×10^{-3}
C_2	0.1419×10^{-4}
C_2H	0.1092×10^{-6}

REFERENCES

I-1. Bird, R. B., W. E. Stewart, and E. N. Lightfoot, Transport Phenomena, New York: John Wiley and Sons, Inc., 1966.

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Santa Monica, California

Reacting Fluids Laboratory

4 Authors

1 Mr. G. Perez