A Numerical Solution of the Navier-Stokes Equations for Chemically Nonequilibrium, Merged Stagnation Shock Layers on Spheres and Two-Dimensional Cylinders in Air

Kenneth D. Johnston and William L. Hendricks

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A Numerical Solution
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<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure</td>
</tr>
<tr>
<td>$c_v$</td>
<td>specific heat at constant volume</td>
</tr>
<tr>
<td>$C_H$</td>
<td>heat transfer coefficient, $\dot{q}<em>w \frac{1}{2} \rho \bar{V}</em>\infty^3$</td>
</tr>
<tr>
<td>$D_{ij}$</td>
<td>binary diffusion coefficient for species pair i and j</td>
</tr>
<tr>
<td>$\bar{e}_i$</td>
<td>specific internal energy of species i</td>
</tr>
<tr>
<td>$\bar{f}_i$</td>
<td>body force on species i per unit mass of species i</td>
</tr>
<tr>
<td>$\bar{h}$</td>
<td>specific enthalpy of mixture</td>
</tr>
<tr>
<td>$\bar{h}_i$</td>
<td>specific enthalpy of species i</td>
</tr>
<tr>
<td>$\bar{k}$</td>
<td>coefficient of thermal conductivity</td>
</tr>
<tr>
<td>$k_{fj}$</td>
<td>forward reaction rate for jth reaction</td>
</tr>
<tr>
<td>$k_{rj}$</td>
<td>reverse reaction rate for jth reaction</td>
</tr>
<tr>
<td>$K_{n\infty}$</td>
<td>freestream Knudsen number, $\frac{\bar{\lambda}_\infty}{\bar{r}_b}$</td>
</tr>
<tr>
<td>$K^2$</td>
<td>hypersonic similarity parameter [see equation (62)]</td>
</tr>
<tr>
<td>$\text{Le}_{ij}$</td>
<td>Lewis number of species pair i and j, $\frac{\rho D_{ij} \bar{c}_p}{\bar{k}}$</td>
</tr>
<tr>
<td>$M_{\infty}$</td>
<td>freestream Mach number</td>
</tr>
<tr>
<td>$M$</td>
<td>indicates a catalyst</td>
</tr>
<tr>
<td>$\text{NS}$</td>
<td>number of species in gas mixture</td>
</tr>
<tr>
<td>$n$</td>
<td>dimensionless radial distance from the body, $(\bar{r} - \bar{r}_b) / \bar{r}_b$</td>
</tr>
<tr>
<td>$n_\infty$</td>
<td>dimensionless radial distance from body to freestream edge (shock layer thickness)</td>
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<table>
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<tr>
<td>$\bar{P}$</td>
<td>pressure</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number, $\bar{C}_p \mu / k$</td>
</tr>
<tr>
<td>$\bar{q}$</td>
<td>heat flux vector</td>
</tr>
<tr>
<td>$\bar{q}_w$</td>
<td>heat flux to wall</td>
</tr>
<tr>
<td>$\bar{r}$</td>
<td>radial distance from body center (see Fig. 1)</td>
</tr>
<tr>
<td>$\bar{r}_b$</td>
<td>radius of body</td>
</tr>
<tr>
<td>$\bar{R}_i$</td>
<td>gas constant of species $i$</td>
</tr>
<tr>
<td>$\bar{R}$</td>
<td>gas constant of mixture</td>
</tr>
<tr>
<td>$\bar{\sigma}$</td>
<td>universal gas constant</td>
</tr>
<tr>
<td>$Re_{0\infty}$</td>
<td>freestream stagnation Reynolds number, $\bar{\rho}<em>\infty \bar{V}</em>\infty \bar{r}<em>b / \bar{\mu}</em>{0\infty}$</td>
</tr>
<tr>
<td>$\bar{S}_{ij}$</td>
<td>collision cross section for particle $i$ with particle $j$</td>
</tr>
<tr>
<td>$Sc_{ij}$</td>
<td>Schmidt number for species pair $i$ and $j$, $\bar{\mu} / \bar{\rho} \bar{D}_{ij}$</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
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<tr>
<td>$T_{0\infty}$</td>
<td>freestream stagnation temperature</td>
</tr>
<tr>
<td>$\bar{t}$</td>
<td>time</td>
</tr>
<tr>
<td>$\bar{u}$</td>
<td>velocity component parallel to body surface (see Fig. 1)</td>
</tr>
<tr>
<td>$\bar{v}$</td>
<td>velocity component normal to body surface (see Fig. 1)</td>
</tr>
<tr>
<td>$\bar{v}$</td>
<td>specific volume of gas mixture</td>
</tr>
<tr>
<td>$\bar{\bar{v}}$</td>
<td>velocity vector</td>
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<td>$\bar{V}_\infty$</td>
<td>freestream speed</td>
</tr>
<tr>
<td>$\bar{V}_i$</td>
<td>diffusion velocity vector of species $i$</td>
</tr>
<tr>
<td>$W_i$</td>
<td>molecular weight of species $i$</td>
</tr>
<tr>
<td>$W$</td>
<td>equivalent molecular weight of mixture</td>
</tr>
<tr>
<td>$\dot{w}_i$</td>
<td>net mass production rate of species $i$ per unit volume</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>mass fraction of species $i$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>ratio of specific heats, $C_p/C_v$</td>
</tr>
<tr>
<td>$\gamma_i$</td>
<td>recombination coefficient for species $i$</td>
</tr>
<tr>
<td>$\eta$</td>
<td>dimensionless radial distance from body surface [see Fig. 1 and equation (24)]</td>
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<tr>
<td>$\Theta_{vi}$</td>
<td>characteristic temperature for vibration of diatomic species $i$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>circumferential angle (see Fig. 1)</td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>mean free path of species $i$</td>
</tr>
<tr>
<td>$\lambda_\infty$</td>
<td>freestream mean free path</td>
</tr>
<tr>
<td>$\mu$</td>
<td>coefficient of absolute viscosity</td>
</tr>
<tr>
<td>$\mu_{SU}$</td>
<td>Sutherland coefficient of absolute viscosity</td>
</tr>
<tr>
<td>$\mu_{0\infty}$</td>
<td>coefficient of absolute viscosity at $T_{0\infty}$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density of mixture</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>molecule-surface accommodation coefficient</td>
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<thead>
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<tr>
<td>( \tau )</td>
<td>viscous stress tensor</td>
</tr>
<tr>
<td>( \Phi )</td>
<td>viscous dissipation function</td>
</tr>
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Subscripts

- \( i, j \) species indices
- \( 0 \) (zero) stagnation condition
- \( s \) edge of Knudsen layer, slip
- \( sh \) conditions behind normal shock
- \( w \) wall
- \( \infty \) freestream property

Superscript

- \( (\cdot) \) dimensional quantity
A NUMERICAL SOLUTION OF THE NAVIER-STOKES EQUATIONS
FOR CHEMICALLY NONEQUILIBRIUM, MERGED STAGNATION
SHOCK LAYERS ON SPHERES AND TWO-DIMENSIONAL
CYLINDERS IN AIR

SUMMARY

The complete Navier-Stokes equations are solved along the stagnation streamline in merged stagnation shock layers on spheres and two-dimensional cylinders using an iterative finite-difference numerical procedure known as the accelerated successive replacement method. The fluid medium is chemically reacting air consisting of seven species. Velocity components, thermodynamic properties, species mass fractions, and wall heat transfer rates are computed. This report is intended as an explanation of the method and as a user's manual for the computer program.

1. INTRODUCTION

An aerospace vehicle ascending or descending through the Earth's atmosphere traverses several flow regimes from the continuum boundary layer regime at low altitudes, through the transitional regime at intermediate altitudes, to the free molecular regime at very high altitudes. The character of the flow field changes drastically from the boundary layer regime to the free molecular regime, and no single computational approach is valid throughout this range. The broad transitional regime may be divided into several sub-regimes as suggested by Hayes and Probstein [1]. Consider the typical spherical nose of an aerospace vehicle. In the boundary layer regime viscous effects are primarily confined to a thin boundary layer, the bow shock can be treated as a discontinuity, and a region of inviscid flow exists between the shock and the boundary layer. However with increasing altitude, the shock wave and boundary layer thicken and eventually merge into a single viscous layer called the shock layer. The flow regime in which this occurs is called the fully merged shock layer regime which is the condition treated in this report.
At the great speed that a vehicle reenters the atmosphere, the temperature near the body becomes extremely high, especially in the stagnation region. Therefore, the air in the shock layer dissociates and ionizes. For an accurate description of the flow field, one must account for these real gas effects. Also an accurate estimate of the ionization level is needed for radio communication purposes. Therefore, a flow field model including finite rate chemistry is required.

This report describes a method for computing flow properties along the stagnation streamlines of a sphere and a circular cylinder transverse to the flow. Heat transfer rates are computed at the body surface. Although this method is limited to the stagnation region, it still provides valuable design information because maximum heating rates usually occur at the nose. The computational method was developed by Jain and Adimurthy [21] for an ideal gas. The method uses the full Navier-Stokes equations to describe the flow in the entire shock layer from the surface to the freestream. The boundary conditions at the wall are provided by slip velocity and temperature jump equations. Using the concept of local similarity, the governing equations are reduced to a system of nonlinear, coupled ordinary differential equations. Numerical solutions are obtained for points on the stagnation streamline using an iterative finite-difference procedure known as the accelerated successive replacement method. The applicability of this approach and the failure of thin-layer theories for the merged shock layer regime is discussed in Reference 2. Nonequilibrium chemical reactions were included in this method by Kumar and Jain [31] using an air model with seven species and six reactions. Hendricks [4] developed surface slip velocity and temperature jump equations for a multi-component gas, including the effects of wall catalysis, to use with this model. Additional modifications have been made in this report, principally by including the two-dimensional cylindrical geometry and using a multi-component gas model to compute viscosity.

II. ANALYSIS

A. Formulation of the Problem

1. Approach. In the present analysis the full Navier-Stokes equations, with nonequilibrium chemistry, are solved through the merged stagnation shock layer from the freestream to the body. The slip conditions at the gas-wall interface include the effect of wall catalysis and a multicomponent, nonequilibrium gas flow.
The thin shock layer assumption is not made in the present analysis. The full Navier-Stokes equations with chemically-reacting, nonequilibrium air are solved through the merged shock and boundary layer. This allows the shock wave to develop within the computational domain. A seven species air model is used. The species considered are N\(_2\), O\(_2\), NO, N, O, NO\(^+\), and e\(^-\). For air dissociation and ionization, the rate expressions recommended by Wray \([5]\) are adopted. Prandtl number, \(Pr\), and Lewis number, \(Le\), are taken to be 0.75 and 1.4, respectively, for the cases computed in this report. The viscosity of dissociated and ionized air is obtained from a simple summation formula for a mixture of hard spherical molecules using Hansen's collision cross sections \([6]\).

Solutions are obtained by using the local similarity concept to reduce the governing equations to a set of nonlinear, coupled, ordinary differential equations. This set of equations is integrated using a finite difference method known as the accelerated successive replacement method. It is important to note that the first order local similarity assumption is a good approximation near the stagnation streamline, at least for \(Re_{sh} \geq 10\) \([7]\). Reference 7 gives a thorough discussion of local similarity.

2. Governing Equations. The nonlinear, coupled ordinary differential equations governing the flow of a multicomponent gas near the stagnation streamlines of spheres and two-dimensional cylinders are presented. The coordinate system employed is shown in Figure 1a.

a. Basic Equations. The basic conservation equations and the ideal gas equation of state for a multicomponent, reacting gas mixture are as follows \([8]\):

Global Continuity (of all species):

\[
\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{v}) = 0 \tag{1}
\]

Species Continuity:

\[
\frac{\partial \bar{N}_i}{\partial t} = \frac{D}{Dt} \bar{N}_i = \frac{\partial \bar{N}_i}{\partial \bar{Y}_i} - \nabla \cdot (\bar{\rho} \bar{Y}_i \bar{V}_i) \quad i = 1, \ldots, NS \tag{2}
\]

where \(NS\) = number of species in mixture (no summation on repeated indices).
Figure 1a. Dimensional coordinate system.

Figure 1b. Dimensionless coordinate system.

Figure 1. Coordinate systems.
Momentum:

\[ \rho \frac{D \vec{v}}{Dt} = -\nabla \vec{P} - \nabla \cdot \vec{\tau} + \bar{\rho} \sum_{i=1}^{NS} Y_i \vec{f}_i \] . \hspace{1cm} (3)

The second order tensor, \( \vec{\tau} \), is the viscous stress tensor and \( \vec{f}_i \) is the body force per unit mass of species \( i \).

Enthalpy:

\[ \rho \frac{D \vec{h}}{Dt} = \frac{D \vec{P}}{Dt} + \vec{\Phi} - \nabla \cdot \vec{q} \] . \hspace{1cm} (4)

The quantity \( \vec{\Phi} \) is the viscous dissipation function and \( \vec{q} \) is the heat flux vector.

State:

\[ \vec{P} = \bar{\rho} \bar{\rho} \bar{T} \sum_{i=1}^{NS} \frac{Y_i}{W_i} \] . \hspace{1cm} (5)

b. Nondimensional Equations. The basic equations are put in non-dimensional form by introducing dimensionless variables as follows:

\[ u = \bar{u}/\bar{V}_\infty \] ,

\[ v = \bar{v}/\bar{V}_\infty \] ,

\[ \rho = \bar{\rho}/\bar{\rho}_\infty \] ,

\[ T = \bar{T}/T_0\infty \] ,
\begin{align*}
\text{P} &= \frac{\overline{P}}{\overline{\rho_\infty}} \overline{V}_\infty^2, \\
h &= \frac{\overline{h}}{\overline{V}_\infty^2}, \\
\mu &= \frac{\overline{\mu}}{\overline{\mu}_0\infty}, \\
r &= \frac{\overline{r}}{\overline{r}_b}, \\
\dot{w}_i &= \frac{\dot{w}_i}{(\overline{\rho}_\infty \overline{V}_\infty / \overline{r}_b)}.
\end{align*}

where \( \overline{r}_b \) is the radius of the body, \( \overline{T}_0\infty \) is the freestream stagnation temperature, and \( \overline{\mu}_0\infty \) is the coefficient of absolute viscosity evaluated at \( \overline{T}_0\infty \). The nondimensional similarity parameters

\begin{equation*}
\text{Re}_{0\infty} = \frac{\overline{\rho}_\infty \overline{V}_\infty \overline{r}_b}{\overline{\mu}_0\infty},
\end{equation*}

\begin{equation*}
\text{Pr} = \frac{\overline{C}}{\overline{p}} \frac{\overline{\mu}}{\overline{k}},
\end{equation*}

\begin{equation*}
\text{Sc}_{ij} = \frac{\overline{\mu}}{\overline{\rho}} \overline{D}_{ij},
\end{equation*}

and

\begin{equation*}
\text{Le}_{ij} = \frac{\overline{k}}{\overline{\rho}} \frac{\overline{C}}{\overline{p}} \overline{D}_{ij}
\end{equation*}

are also introduced. The basic equations are then simplified by assuming steady flow and Newtonian fluid, neglecting body forces, viscous diffusion stresses, thermal radiation, and thermal diffusion, and using Fick's Law of Diffusion. The equations are presented in cylindrical and spherical coordinates below.
Cylindrical Coordinates:

Global Continuity:

\[
\frac{\partial}{\partial r} (\rho v_r) + \frac{\partial}{\partial \theta} (\rho u) = 0 \quad . \tag{6}
\]

Species Continuity:

\[
\rho \left( v \left( \frac{\partial Y_i}{\partial r} + \frac{u}{r} \frac{\partial Y_i}{\partial \theta} \right) \right) = \dot{\bar{\omega}}_i + \frac{1}{\text{Re}_0} \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( \frac{\mu r}{Sc} \frac{\partial Y_i}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{\mu r}{Sc} \frac{\partial Y_i}{\partial \theta} \right) \right] . \quad i = 1, \ldots, \text{NS} \tag{7}
\]

Transverse Momentum (\(\theta\) Direction):

\[
\rho \left( v \frac{\partial u}{\partial r} + \frac{u}{r} \frac{\partial u}{\partial \theta} + \frac{vu}{r} \right) = -\frac{1}{r} \frac{\partial P}{\partial \theta} + \frac{1}{\text{Re}_0} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \left[ \frac{\partial}{\partial r} \left( \frac{u}{r} \right) + \frac{1}{r} \frac{\partial v}{\partial \theta} \right] \right) \right] \tag{8}
\]

Radial Momentum (r Direction):

\[
\rho \left( v \frac{\partial v}{\partial r} + \frac{u}{r} \frac{\partial v}{\partial \theta} - \frac{u^2}{r} \right) = -\frac{\partial P}{\partial r} + \frac{1}{\text{Re}_0} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \left[ \frac{\partial}{\partial r} \left( \frac{2}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right) - \frac{2}{3} \left[ \frac{1}{r} \frac{\partial}{\partial r} (rv) + \frac{1}{r} \frac{\partial u}{\partial \theta} \right] \right] \right) \right] . \tag{9}
\]
Enthalpy:

\[ \rho \left( v \frac{\partial h}{\partial r} + \frac{u}{r} \frac{\partial h}{\partial \theta} \right) = v \frac{\partial P}{\partial r} + \frac{u}{r} \frac{\partial P}{\partial \theta} + \frac{\mu}{Re_0} \left[ 2 \left( \frac{\partial v}{\partial r} \right)^2 + \left( \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right)^2 \right] \]

\[ + \left( \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial u}{\partial r} \left( \frac{\partial u}{\partial \theta} - \frac{u}{r} \right) \right) - \frac{2 \mu}{3 Re_0} \left[ \frac{\partial v}{\partial r} + \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right]^2 \]

\[ + \frac{1}{Pr Re_0} \left\{ \frac{\partial}{\partial r} \left( \frac{\mu}{Pr} \frac{\partial h}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{\mu}{r} \frac{\partial h}{\partial \theta} \right) \right\} \]

\[ + (Le - 1) \frac{\partial}{\partial r} \left[ \sum_{i=1}^{NS} r \mu h_i \frac{\partial Y_i}{\partial r} \right] + (Le - 1) \frac{\partial}{\partial \theta} \left[ \sum_{i=1}^{NS} \frac{\mu h_i}{r} \frac{\partial Y_i}{\partial \theta} \right] \right\} . \]

(10)

State:

\[ P = \rho \bar{T} \frac{\bar{T}^{0\infty}}{V^2} \sum_{i=1}^{NS} \frac{Y_i}{W_i} . \]

(11)

Spherical Coordinates:

Global Continuity:

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( \rho r^2 v \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \rho u \sin \theta \right) = 0 . \]

(12)
Species Continuity:

$$\rho \left( \frac{\partial Y_i}{\partial r} + u \frac{\partial Y_i}{\partial \theta} \right) = \frac{\hat{w}_i}{Re_{\infty}} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{r^2 \mu}{Sc} \frac{\partial Y_i}{\partial r} \right) \right. $$

$$\left. + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \frac{\mu \sin \theta}{Sc} \frac{\partial Y_i}{\partial \theta} \right) \right] \quad i = 1, \ldots, NS \ (13)$$

Transverse Momentum ($\theta$ Direction):

$$\rho \left( \frac{\partial u}{\partial r} + \frac{u^2}{r} + u \frac{\partial u}{\partial \theta} \right) = -\frac{1}{r} \frac{\partial P}{\partial \theta} + \frac{1}{Re_{\infty}} \left\{ \frac{\partial}{\partial r} \left[ \mu \frac{\partial}{\partial r} \left( \frac{u}{r} \right) + \frac{u}{r} \frac{\partial v}{\partial \theta} \right] \right.$$ 

$$+ \frac{1}{r^2} \frac{\partial}{\partial \theta} \left[ \frac{4}{3} \mu \left( \frac{\partial u}{\partial \theta} + v \right) - \frac{2}{3} \mu \left( r \frac{\partial^2 v}{\partial r^2} + v + u \cot \theta \right) \right]$$

$$\left. + \frac{3}{r} \mu \left[ r \frac{\partial}{\partial r} \left( \frac{u}{r} \right) + \frac{1}{r} \frac{\partial v}{\partial \theta} \right] + \frac{2}{r^2} \mu \cot \theta \left[ \frac{\partial u}{\partial \theta} - u \cot \theta \right] \right\} \quad . \ (14)$$

Radial Momentum ($r$ Direction):

$$\rho \left( \frac{\partial v}{\partial r} + \frac{u^2}{r} + \frac{\partial v}{\partial \theta} - \frac{u^2}{r} \right) = -\frac{\partial P}{\partial r} + \frac{1}{Re_{\infty}} \left\{ \frac{\partial}{\partial r} \left[ \frac{4}{3} \mu \frac{\partial v}{\partial r} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial \theta} + 2v + u \cot \theta \right) \right] \right.$$ 

$$\left. + \frac{1}{r} \frac{\partial}{\partial \theta} \left[ \mu r \frac{\partial}{\partial r} \left( \frac{u}{r} \right) + u \frac{\partial v}{\partial \theta} \right] + \frac{4}{r^2} \mu \frac{\partial v}{\partial r} - \frac{v}{r} \right.$$ 

$$\left. - \frac{\mu}{r^2} \left[ 2 \frac{\partial u}{\partial \theta} + 2u \cot \theta - r^2 \cot \theta \frac{\partial}{\partial r} \left( \frac{u}{r} \right) - \frac{\partial v}{\partial \theta} \cot \theta \right] \right\} \quad . \ (15)$$
Enthalpy:

\[
\rho \left( v \frac{\partial h}{\partial r} + u \frac{\partial h}{\partial \theta} \right) = v \frac{\partial P}{\partial r} + u \frac{\partial P}{\partial \theta} + \frac{\mu}{\text{Re}_0} \left[ 2 \left( \frac{\partial v}{\partial r} \right)^2 + \left( \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right)^2 \right] + \left( \frac{v}{r} + \frac{u \cot \theta}{r} \right)^2 + \left[ \frac{1}{r} \frac{\partial v}{\partial \theta} + r \frac{\partial}{\partial r} \left( \frac{u}{r} \right) \right]^2 - \frac{2}{3} \frac{\mu}{\text{Re}_0} \left[ \frac{\partial v}{\partial r} + \frac{1}{r} \frac{\partial u}{\partial \theta} \right] \]

\[
+ \frac{2v}{r} + \frac{u \cot \theta}{r} \right]^2 + \frac{1}{\text{Re}_0 \text{Pr}} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( \mu r^2 \frac{\partial h}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{\mu \sin \theta \partial h}{r} \right) \right] + (\text{Le} - 1) \frac{1}{r^2} \frac{\partial}{\partial r} \sum_{i=1}^{\text{NS}} \left( \mu r^2 h_i \frac{\partial Y_i}{\partial r} \right) \]

\[
+ (\text{Le} - 1) \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \sum_{i=1}^{\text{NS}} \left( \frac{\partial h_i}{r} \frac{\sin \theta}{\partial \theta} \frac{\partial Y_i}{\partial \theta} \right) \right] . \tag{16}
\]

State:

\[
P = \rho T \frac{\bar{S}_0}{\bar{V}_0} \sum_{i=1}^{\text{NS}} \frac{Y_i}{W_i} \quad . \tag{17}
\]

In the previous equations, Le\(_{ij}\) is assumed to be the same for all species pairs i,j and is, therefore, replaced with Le. Similarly, Sc\(_{ij}\) is replaced with Sc.

The local similarity approximation for the zone near the axis of symmetry is given by equations (18) through (24). The validity of this approximation was demonstrated by Kao [7].
\[ u(r, \theta) = u_1(r) \sin \theta \quad (18) \]

\[ v(r, \theta) = v_1(r) \cos \theta \quad (19) \]

\[ h(r, \theta) = h_1(r) \quad (20) \]

\[ \rho(r, \theta) = \rho_1(r) \quad (21) \]

\[ P(r, \theta) = P_1(r) + P_2(r) \sin^2 \theta \quad (22) \]

\[ \mu(r, \theta) = \mu_1(r) \quad (23) \]

\[ Y_i(r, \theta) = Y_{1i}(r) \quad . \quad (24) \]

Equations (18) through (24) are used to reduce the governing equations to a set of nonlinear, coupled, ordinary differential equations which can be solved rapidly.

A transformation is now made in the normal coordinate by defining

\[ \eta = \frac{r - 1}{r_\infty - 1} = \frac{n}{n_\infty} \quad , \quad (25) \]

where \( r_\infty \) is the nondimensional distance from the origin to the freestream and \( n_\infty \) is the nondimensional distance from the body to the freestream (Fig. 1b). The values of \( r_\infty \) and \( n_\infty \) are unknown a priori. They are determined as part of the solution. This transformation, equation (25), keeps the body at \( \eta = 0 \) and the freestream at \( \eta = 1 \).

By substituting equations (18) through (25) into the governing equations and equating the coefficients of like functions of \( \theta \), one obtains the following system of ordinary differential equations:
Cylindrical Coordinates:

\[
\frac{\rho_1'}{\rho_1} = -\frac{v_1'}{v_1} - \frac{n_\infty}{1 + \eta n_\infty} \left(1 + \frac{u_1}{v_1}\right) \quad . \quad (26)
\]

\[
\frac{u_1''}{n_\infty^2} = \frac{\text{Re}_{0\infty} \rho_1}{\mu_1} \left(\frac{v_1 u_1'}{n_\infty} + \frac{u_1^2 + u_1 v_1}{1 + \eta n_\infty}\right) + \frac{2 \text{P}_2 \text{Re}_{0\infty}}{\mu_1 (1 + \eta n_\infty)}
+ \frac{u_1 + v_1}{(1 + \eta n_\infty)} \left[\frac{\mu_1'}{\mu_1 n_\infty} + \frac{7}{3(1 + \eta n_\infty)}\right]
- \frac{u_1'}{n_\infty} \left(\frac{2}{1 + \eta n_\infty} + \frac{\mu_1'}{\mu_1 n_\infty}\right)
+ \frac{v_1'}{3n_\infty (1 + \eta n_\infty)} \quad . \quad (27)
\]

\[
\frac{v_1''}{n_\infty^2} = \frac{3 \text{Re}_{0\infty}}{4 n_\infty \mu_1} \left(P_1' + \rho_1 v_1 v_1'\right) - \frac{v_1'}{n_\infty} \left(\frac{\mu_1'}{\mu_1 n_\infty} + \frac{1}{1 + \eta n_\infty}\right)
- \frac{u_1'}{4n_\infty (1 + \eta n_\infty)}
+ \frac{(u_1 + v_1)}{1 + \eta n_\infty} \left[\frac{\mu_1'}{2\mu_1 n_\infty} + \frac{7}{4(1 + \eta n_\infty)}\right] \quad . \quad (28)
\]

\[
\frac{P_2'}{n_\infty} = \frac{P_1'}{n_\infty} + \frac{\rho_1 u_1}{1 + \eta n_\infty} (u_1 + v_1) \quad . \quad (29)
\]
\[
\frac{\rho_1 v_{11} h'_1}{n_\infty} (1 + \eta n_\infty)^2 = (1 + \eta n_\infty)^2 \left[ \frac{v_{11}}{n_\infty} + \frac{2 \mu_1}{Re_{\infty}} \frac{v_{11}^2}{n_\infty^2} \right] + \frac{2 \mu_1}{Re_{\infty}} (u_1 + v_1)^2
\]

\[
- \frac{2}{3} \frac{\mu_1}{Re_{\infty}} \left[ \frac{(1 + \eta n_\infty)}{n_\infty} v_1' + (u_1 + v_1) \right]^2
\]

\[
= \frac{(1 + \eta n_\infty)}{Re_{\infty} \Pr n_\infty} \left\{ \mu_1 h'_1 + \frac{(1 + \eta n_\infty)}{n_\infty} (h'_1 \mu'_1 + \mu_1 h''_1) \right. \\
+ (Le - 1) \left[ \left( \mu_1 + \frac{\mu'_1 (1 + \eta n_\infty)}{n_\infty} \right)^{NS} \sum_{i=1}^{NS} h_i Y''_{i1} \right. \\
\left. + \frac{\mu_1 (1 + \eta n_\infty)}{n_\infty} \sum_{i=1}^{NS} (h'_i Y'_{i1} + h_i Y''_{i1}) \right]\right\} . \tag{30}
\]

\[
\frac{\rho_1 v_{11} Y'_{i1}}{n_\infty} = \dot{W}_i + \frac{1}{(1 + \eta n_\infty) Re_{\infty} \Sc} \left[ \frac{\mu_1 Y'_{i1}}{n_\infty} + \frac{\mu'_1 Y''_{i1}}{n_\infty} (1 + \eta n_\infty) \right. \\
+ \frac{\mu_1 (1 + \eta n_\infty)}{n_\infty^2} Y''_{i1} \right] \quad i = 1, \ldots, NS \tag{31}
\]

\[
P_1 = \rho_1 T_1 \sum_{i=1}^{NS} \left( \frac{Y_{i1}}{\hat{V}_{i\infty}^2} \right) \quad \left( \sum_{i=1}^{NS} \frac{Y_{i1}}{W_i} \right) \quad \tag{32}
\]

Here, a prime denotes differentiation with respect to \( \eta \).
Spherical Coordinates:

\[ \rho_1' \rho_1 = -\frac{v_1'}{v_1} - \frac{2n_\infty}{1 + \eta n_\infty} \left(1 + \frac{u_1}{v_1}\right) \quad (33) \]

\[ \frac{u_1'''}{n_\infty^2} = \frac{\text{Re}_{0\infty} \rho_1}{\mu_1} \left(\frac{v_1 u_1'}{n_\infty} + \frac{u_1'^2 + u_1 v_1}{1 + \eta n_\infty}\right) + \frac{2P_2 \text{Re}_{0\infty}}{\mu_1 (1 + \eta n_\infty)} \]

\[ + \frac{u_1 + v_1}{(1 + \eta n_\infty)} \left[\frac{\mu_1'}{\mu_1 n_\infty} + \frac{8}{3(1 + \eta n_\infty)}\right] - \frac{u_1'}{n_\infty} \left(\frac{2}{1 + \eta n_\infty} + \frac{\mu_1'}{\mu_1 n_\infty}\right) \]

\[ + \frac{v_1'}{3n_\infty (1 + \eta n_\infty)} \cdot \quad (34) \]

\[ \frac{v_1'''}{n_\infty^2} = \frac{3}{4} \frac{\text{Re}_{0\infty}}{n_\infty \mu_1} \left(P_1' + \rho_1 v_1 v_1\right) - \frac{v_1'}{n_\infty} \left(\frac{\mu_1'}{\mu_1 n_\infty} + \frac{2}{1 + \eta n_\infty}\right) - \frac{u_1'}{2n_\infty (1 + \eta n_\infty)} \]

\[ + \frac{(u_1 + v_1)}{(1 + \eta n_\infty)} \left[\frac{\mu_1'}{\mu_1 n_\infty} + \frac{7}{2(1 + \eta n_\infty)}\right] \cdot \quad (35) \]

\[ \frac{P_2'}{n_\infty} = -\frac{P_1'}{n_\infty} + \frac{\rho_1 u_1}{1 + \eta n_\infty} (u_1 + v_1) \quad . \quad (36) \]
\[
\frac{p_1 v_1 h'_1}{n_\infty} (1 + \eta n_\infty)^2 = (1 + \eta n_\infty)^2 \left[ \frac{v_1 P'_1}{n_\infty} + \frac{2\mu_1}{Re_\infty} \frac{v'^2_1}{n_\infty^2} \right] + \frac{4\mu_1}{Re_\infty} (u_1 + v_1)^2
\]

\[
- \frac{2}{3} \frac{\mu_1}{Re_\infty} \left[ \frac{(1 + \eta n_\infty)}{n_\infty} v'_1 + 2 (u_1 + v_1) \right]^2
\]

\[
+ \frac{(1 + \eta n_\infty)}{Re_\infty Pr n_\infty} \left\{ \frac{2\mu_1 h'_1}{n_\infty} + \frac{(1 + \eta n_\infty)}{n_\infty} (\mu'_1 h'_1 + \mu''_1 h'_1) \right\}
\]

\[
+ (Le - 1) \left[ \left( 2 \mu_1 + \frac{\mu'_1 (1 + \eta n_\infty)}{n_\infty} \right) \sum_{i=1}^{NS} h'_1 Y'_{1i} \right. \]

\[
+ \frac{\mu_1 (1 + \eta n_\infty)}{n_\infty^2} \left( \sum_{i=1}^{NS} (h'_1 Y'_{1i} + h'_1 Y''_{1i}) \right) \left. \right\}
\]

\[
\frac{\rho_1 v_1 Y'_{1i}}{n_\infty} = \dot{w}_i + \frac{1}{(1 + \eta n_\infty) Re_\infty Sc} \left[ 2\mu_1 Y'_{1i} + \frac{\mu_1 Y'_{1i}}{n_\infty^2} (1 + \eta n_\infty) \right. \]

\[
\left. + \frac{\mu_1 (1 + \eta n_\infty) Y''_{1i}}{n_\infty^2} \right] \quad i = 1, \ldots, NS
\]

\[
P_1 = \rho_1 T_1 \frac{\bar{\Delta} T_{0\infty}}{V_\infty^2} \sum_{i=1}^{NS} \left( \frac{Y_{1i}}{W_{1i}} \right)
\]
Equations (26) through (32) and (33) through (39) constitute two sets of non-linear ordinary differential equations for cylindrical and spherical stagnation regions, respectively. Each of these sets contain 6 + NS equations and 8 + 2NS unknowns ($\mu_1, v_1, P_1, P_2, \rho_1, T_1, h_1, \mu_1, \dot{w}_1$, and $Y_{11}$). The required additional information and equations are given below for the mass production rates, $\dot{w}_1$, enthalphy, $h_1$, and viscosity, $\mu_1$, of a dissociated and ionized air mixture. These equations, like the equation of state above, are independent of the coordinate system.

c. Air Chemistry. The freestream air is assumed to consist of $N_2$ and $O_2$ molecules only. The air model used for the shock layer consists of seven species and the seven chemical reactions as follows [5]:

\[
\begin{align*}
O_2 + M + 5.1 \text{ eV} & \xrightleftharpoons{k_{r1}} O + O + M \\
N_2 + M + 9.8 \text{ eV} & \xrightleftharpoons{k_{r2}} N + N + M \\
NO + M + 6.5 \text{ eV} & \xrightleftharpoons{k_{r3}} N + O + M \\
NO + O + 1.4 \text{ eV} & \xrightleftharpoons{k_{r4}} O_2 + N \\
N_2 + O + 3.3 \text{ eV} & \xrightleftharpoons{k_{r5}} NO + N \\
N_2 + O_2 + 1.9 \text{ eV} & \xrightleftharpoons{k_{r6}} NO + NO
\end{align*}
\]
\[
\begin{align*}
\frac{k_{f7}}{k_{r7}}N + O + 2.8 \text{ eV} & \xrightleftharpoons{} \text{ NO}^+ + e^- . \\
\end{align*}
\]

These reactions are written so that the forward reactions are endothermic; the net amounts of energy required to produce the reactions are given on the left side of the equations. The first three reactions are the neutral-particle dissociation-recombination reactions in which the energy of dissociation in the forward reaction is taken primarily from kinetic energy by means of a collision with a "catalytic" molecule M; the chemical energy released in the recombination (reverse reaction) is converted primarily to kinetic energy in a three-body collision involving a catalytic molecule M. The M molecule can be any of the six molecular or atomic species present in the air mixture. The quantities \(k_{fj}\) and \(k_{rj}\) are the temperature-dependent forward and reverse reaction rates, respectively, for the jth reaction. The experimentally determined reaction rates recommended by Wray [5] are used, together with the concentrations of all constituents, to obtain the mass production rates, \(\dot{w}_i\), of each constituent [9]. The reader is referred to Reference 10 for details.

d. Enthalpy. The specific enthalpy of a mixture of gases is given in dimensional form as follows:

\[\bar{h} = \bar{P} \bar{v} + \sum_{i=1}^{NS} Y_i \bar{e}_i, \quad (40)\]

where

\[\bar{e}_i = \bar{e}_i^0 + \bar{e}_{T_i} + \bar{e}_{R_i} + \bar{e}_{v_i}, \quad (41)\]

and

\[\bar{e}_i^0 = \text{ specific energy of formation of species } i \text{ at the reference temperature (zero absolute)}\]

\[\bar{e}_{T_i} = \text{ specific energy of random translation}\]
\( \tilde{e}_{R_i} = \) specific energy of rotation (for diatomic molecule)
\( \tilde{e}_{V_i} = \) specific energy of vibration (for diatomic molecules).

We assume that the energy of electronic excited states is negligible, that the rotational state is fully excited, but that the vibrational state is partially excited. Values for these quantities are given by Vincenti and Kruger [9]:

\[
\tilde{e}_{T_i} = \frac{3}{2} \tilde{R}_i \tilde{T} \tag{42}
\]

\[
\tilde{e}_{R_i} = \tilde{R}_i \tilde{T} \tag{43}
\]

\[
\tilde{e}_{V_i} = \left( \tilde{R}_i \Theta_{V_i} \right) \frac{\Theta_{V_i} / \tilde{T}}{1} \tag{44}
\]

where

\( \Theta_{V_i} = \) characteristic temperature for vibration of diatomic species \( i \)
\( \Theta_{V_{O2}} = 2270 \text{ K} \)
\( \Theta_{V_{N2}} = 3390 \text{ K} \)
\( \Theta_{V_{NO}} = 2740 \text{ K} \)
\( \Theta_{V_{NO^+}} = 2740 \text{ K} \).
Equation (40) now becomes

\[ \bar{h} = \frac{5}{2} \frac{\bar{\Theta}}{T} \sum_{i=1}^{\text{NS}} \frac{Y_i}{W_i} + \bar{\Theta} \sum_{i=1}^{\text{NS}} \frac{Y_i}{W_i} \left( \frac{\bar{\Theta} v_i}{\Theta v_i / T} \right) e^{\Theta v_i / T} - 1 \]

(for diatomic molecules)

Nondimensionalizing equation (45), we obtain

\[ h = \frac{5}{2} \frac{\bar{\Theta} T_0}{V_\infty^2} \sum_{i=1}^{\text{NS}} \frac{Y_i}{W_i} \frac{\bar{\Theta} T_0}{V_\infty^2} \sum_{i=1}^{\text{NS}} \frac{Y_i}{W_i} \left( \frac{\Theta v_i}{\Theta v_i / T} \right) e^{\Theta v_i / T} - 1 \]

(46)

\[ + \frac{1}{V_\infty^2} \sum_{i=1}^{\text{NS}} Y_i \bar{e}_i^0 \]

Viscosity. The Sutherland formula for the viscosity of air gives acceptable results at moderate temperatures, but it fails at the extremely high temperatures encountered in hypersonic flight. The viscosity begins deviating from the Sutherland value due to the onset of dissociation at approximately 3000 K. The viscosity near the wall is also affected by the extremely low pressures encountered at high altitude [11]. This effect is due to velocity slip at the wall (see next section). The Sutherland formula, equation (47), is recommended for temperatures less than 3000 K.

\[ \bar{\mu}_{su} = \frac{1.458 \times 10^{-5} T^{3/2}}{110.4 + T} \text{ [gm/cm sec]} \]  

\[ \text{[47]} \]

This formula is also used in the computer program (Appendix A) to calculate \( \bar{\mu}_{0\infty} \) using \( T_{0\infty} \) computed from the adiabatic relation for temperature,
although it is realized that neither $\bar{\mu}_{su}$ nor $\bar{T}_{0\infty}$ has valid physical meaning at extremely high stagnation enthalpy. This use is justified because $\bar{\mu}_{0\infty}$ is used only for nondimensionalizing $\bar{\mu}$ and for computing $Re_{0\infty}$.

The viscosity of dissociated and ionized air is approximated in Reference 6 using a simple summation formula for a mixture of hard spherical molecules:

$$\frac{\bar{\mu}}{\bar{\mu}_{su}} = \sum_{i=1}^{NS} \frac{W_i}{Y_i} \sqrt{\frac{\bar{\lambda}_i}{\bar{\lambda}_R}}$$   \hspace{1cm} (48)$$

where

$\bar{\mu}_{su}$ = viscosity at same temperature from Sutherland formula

$W_R$ = equivalent molecular weight of undissociated air

$\bar{\lambda}_i$ = mean free path of species $i$

$\bar{\lambda}_R$ = mean free path of undissociated air molecules.

The ratio of mean free paths in equation (48) is given by

$$\frac{\bar{\lambda}_R}{\bar{\lambda}_i} = \sum_{j=1}^{NS} \frac{W_R}{Y_j} \frac{\bar{S}_{ij}}{\bar{S}_R} \left( \frac{1 + \frac{W_j}{W_i}}{2} \right)^{1/2}$$   \hspace{1cm} (49)$$

where

$\bar{S}_{ij}$ = collision cross section for particle $i$ with particle $j$

$\bar{S}_R$ = collision cross section for undissociated air molecules.

The collision cross sections are tabulated as a function of temperature in Reference 6.
The viscosity given by equation (48) is a function of the composition of the gas mixture and also of the temperature via the dependence of $\tilde{S}_R$ and $\tilde{S}_{ij}$ on temperature. Since in the present analysis the air is not in chemical equilibrium, the viscosity obtained from the computer program at a given temperature differs greatly from that shown in Reference 6 for equilibrium conditions. As the mass fractions of the components of air approach their undissociated values, the numerical value of the viscosity ratio in equation (48) approaches 1.0, i.e., $\mu$ approaches the Sutherland value as expected.

3. **Boundary Conditions.** To solve the governing equations given in the previous section, freestream and wall boundary conditions are required.

Freestream ($\eta = 1$):

The air at the freestream boundary is in its undisturbed state.

\[ u_1 = 1, \]

\[ v_1 = -1, \]

\[ p_1 = 1, \]

\[ T_1 = T_\infty, \]

\[ p_1 = p_\infty, \]

\[ p_2 = 0, \]

\[ Y_{1N_2} = 0.767, \]

\[ Y_{1O_2} = 0.233, \]

\[ Y_{1NO} = Y_{1N} = Y_{1O} = Y_{1NO^+} = Y_{1e^-} = 0. \]
In high-altitude, low-Reynolds number flight, the continuum model of the gas breaks down in regions of large gradients of the physical properties near the wall. Hence, the Navier-Stokes description is invalid for the gas layer near the wall (Knudsen layer) with thickness on the order of the mean free path \[11\]. Also, the familiar continuum zero-velocity and zero-temperature-jump wall boundary conditions are not applicable. Although the Navier-Stokes equations are invalid near the wall, they can still be used, down to quite low Reynolds numbers, to describe the outer flow field if the proper boundary conditions are used at the outer edge of the Knudsen layer. These boundary conditions, known as slip conditions, are the mean velocity, temperature, and species mass fractions. To compute these slip conditions, a kinetic theory approach must be used for the Knudsen layer. The boundary conditions for the Knudsen layer are the mean slip conditions at the outer edge and the kinetic gas-surface conditions at the wall.

The Boltzmann equation is the governing equation for the kinetic theory description of a flow field. However, due to the difficulty in solving the Boltzmann equation for the Knudsen layer, we resorted to an approximate kinetic theory slip model. Reference 4 gives the details of the derivation of the slip conditions for a multicomponent reacting gas. By matching the species, momenta, and energy fluxes at the outer edge of the Knudsen layer to the difference between the incident and reflected fluxes at the wall, the jump in the desired properties across the Knudsen layer is obtained. The fluxes are calculated by taking moments of the velocity distribution function which is approximated by using a Chapman-Enskog expansion for a multicomponent mixture. The species flux is greatly affected by the catalytic nature of the wall. The wall is assumed to be catalytic with respect to recombination of dissociated molecules. Equations are obtained for a partially catalytic wall. The extremes of noncatalytic and fully catalytic walls are easily obtained from the equations for a partially catalytic wall. The resulting nondimensional equations for slip velocity, temperature, and species are as follows:

\[
u_s = \frac{\mu_s}{\rho_w \Re_{\infty} M_{\infty}} \left[ \sqrt{\frac{2}{\pi}} \left( \frac{2}{\sigma} \right) \frac{2T_s}{\sqrt{\gamma T_{\infty}}} \left( \frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} \right) \right]
\]

\[+ \frac{1}{5(\gamma-1) M_{\infty} \Pr_{\infty}} \left( \frac{1}{r} \frac{\partial T}{\partial \theta} \right) \sum_i \sqrt{\frac{W_i}{W}}
\]

\[- \frac{P_w M_{\infty} \Le}{\rho_w \Pr} \sum_j \left( \frac{1}{r} \frac{\partial Y_j}{\partial \theta} \right) \sum_i \sqrt{\frac{W_i}{W}} \right]. \quad (50)\]
The superscript, \( s \), on \( Y^s_i \) denotes the value of \( Y_i \) at the outer edge of the Knudsen layer.
The similarity equations (18) through (24) and the coordinate transformation equation (25) are used in equations (50) through (52) to yield the following slip equations:

\[ u_{ls} = \frac{\mu_{ls}}{P_{lw} Re_\infty M_\infty} \left[ \sqrt{\frac{\pi}{2}} \left( \frac{2 - \sigma}{2\sigma} \right) \sqrt{\frac{2T_1}{\gamma T_\infty}} \left( \frac{u_1}{\eta_{\infty}} \right) \right]_s, \quad (53) \]

\[ T_{ls} = \left( T_w \sum_i \left\{ \frac{\rho_1 Y_{1i}}{W_i \sum_j \frac{Y_{1j}}{W_j}} \cdot \frac{M_\infty}{3P_{11} Re_\infty} \right\} - \left[ 1 + \frac{\mu_1}{3P_{11} Re_\infty} \left( \frac{u_1}{1 + \eta_{\infty}} - \frac{2v_1}{n_{\infty}} \right) \right] \right) \]

\[ + \frac{\sqrt{\pi}}{Y_{1i}} \left( \frac{2 - \sigma}{\sigma} \right) \frac{M_\infty}{Re_\infty} \frac{Le}{Pr} \left[ W_i \sum_j \frac{Y_{1j}}{W_j} \right] \frac{\mu_1}{\rho_1} \sqrt{\frac{\gamma W_i T_\infty}{2WT_1}} \sum_j \frac{Y_{1j}'}{n_{\infty}} \right]_s \]

\[ + \frac{2 - \sigma}{\sigma} \sqrt{\pi} \left[ \frac{M_\infty}{PrRe_\infty} \frac{\gamma - 1}{2} \sqrt{\frac{\gamma T_\infty}{2T_1}} \frac{T_1'}{n_{\infty}} \right] \]

\[ - \frac{5P_{11}}{2\rho_1} \frac{\mu_1}{Re_\infty} M_\infty^3 \gamma T_\infty \sqrt{\frac{\gamma T_\infty}{2T_1}} \frac{Le}{Pr} \sum_j \frac{Y_{1j}'}{n_{\infty}} \right]_s \]

\[ \left\{ \sum_i \left[ \frac{\rho_1 Y_{1i}}{W_i \sum_j \frac{Y_{1j}}{W_j}} \right]^{3/2} \left[ 1 + \frac{\mu_1}{2P_{11} Re_\infty} \left( \frac{u_1}{1 + \eta_{\infty}} - \frac{2v_1}{n_{\infty}} \right) \right] \right\}_s, \quad (54) \]

and

24
The quantity $\gamma_1$ in equation (55) is the recombination coefficient for the $i$ species; it is a measure of the catalyticity of the wall. The value of $\gamma_1$ varies from 0 (noncatalytic wall) to 1 (fully catalytic wall).

The computer program used in this report has the fully catalytic wall and noncatalytic wall options, but it does not, in the present form, have a partially catalytic wall option [for a given catalyticity $\gamma_1$, equation (55) would give $Y_{1i}^S$]. In the fully catalytic wall option, the wall is assumed to be catalytic only with respect to recombination of neutral atomic species; it is assumed to be non-catalytic with respect to recombination of the charged particles $NO^+$ and $e^-$. The wall boundary conditions on $Y_{1i}^S$ for these special cases are given as follows:

Noncatalytic Wall:

For a noncatalytic surface ($\gamma_1 = 0$), equation (55) reduces to

$$\sum_j (Y_{1j}^i)_{S} = 0 \quad .$$

(56)

A sufficient condition for equation (56) to be satisfied is that

$$(Y_{1j}^i)_{S} = 0 \quad j = 1, \ldots, NS \quad .$$

(57)

Equation (57) is also the most physically plausible means by which equation (56) can be satisfied; therefore, equation (57) is taken as the noncatalytic boundary condition for species mass fractions.
Fully Catalytic Wall:

For the fully catalytic wall, the surface is assumed to be fully catalytic with respect to recombination of neutral atomic species, but it is assumed to be noncatalytic with respect to recombination of the charged particles $\text{NO}^+$ and $e^-$. Therefore, the effect of the wall is to drive the gas towards its freestream composition, except for the charged particles $\text{NO}^+$ and $e^-$. The following boundary conditions are then obtained:

\[
\begin{align*}
(Y_{N_2})_s &= 0.767 \\
(Y_{O_2})_s &= 0.233 \\
(Y_{\text{NO}})_s &= (Y_N)_s = (Y_O)_s = 0 \\
(Y'_{\text{NO}^+})_s &= (Y'_{e^-})_s = 0.
\end{align*}
\]

Equations (58), (59), and (61) produce the impossible result that

\[
\sum_{i=1}^{NS} Y_i > 1 ;
\]

however, because $(Y_{\text{NO}^+})_s$ and $(Y_{e^-})_s$ are usually very small, this error is tolerable.

B. Method of Solution

Equations (26) through (32) and (33) through (39) together with equations (46) and (48) constitute two sets of nonlinear, coupled ordinary differential equations with boundary conditions previously given. The first order equations are solved by direct numerical quadrature, and the second order equations are
integrated by a finite difference method known as the successive accelerated replacement method which is an iterative scheme that starts from a guessed solution. The salient feature of this method, proposed by Lieberstein [13], is that the successive corrections applied to the flow profiles in each iteration are controlled by acceleration factors which are used to increase the rate of convergence of the computed quantities. Thus, this method can be successfully applied even if the initial, guessed profiles do not approximate the converged solutions very well. For the present application, this statement holds true in the midrange of the flow regime for which our analysis is applicable. However, divergence problems are encountered at the continuum end of the regime (Appendix A).

C. Computer Program

Details of the computer program are found in Reference 10, while Appendix A is a current users manual.

III. RESULTS

Results from the computer program, with the modifications introduced in this report, are first compared with the "old" program. Then, the program output is compared with some available experimental data. Finally, some general results from the program and input data for running the program are presented.

A. Effect of Computer Program Modifications

The program described as the old program includes all the analysis in this report except the constitutive equations (46) and (48) for enthalpy and viscosity, respectively. The old enthalpy equation assumed a fully excited vibrational state for diatomic molecules. This assumption is always violated near the freestream and near the wall because temperatures in these regions are less than \( T_v \). The old viscosity equation (Sutherland) is restricted to non-dissociated air or to temperatures less than approximately 3000 K at equilibrium conditions. This temperature is greatly exceeded in the central part of the shock layer at reentry speeds.
B. Comparison of Data Between Old Program and Modified Program

Computed values of shock layer thickness, $n_\infty$; wall heat transfer coefficient at the stagnation point, $C_H$; and maximum ratio of viscosity to Sutherland viscosity on the stagnation streamline, $\mu/\mu_{su}$, are given in Table 1 for a 30.5-cm radius sphere using (1) the "old" program, (2) the program with enthalpy modification only, and (3) the program with enthalpy and viscosity modifications. The conditions for which the runs were made are listed in Table 1. The thermodynamic properties associated with altitude are obtained throughout this report from Reference 14.

<table>
<thead>
<tr>
<th>Program Identification</th>
<th>Shock Layer Thickness $n_\infty$</th>
<th>Wall Heat Transfer Coefficient $C_H$</th>
<th>$(\mu/\mu_{su})_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Old Program</td>
<td>0.1361</td>
<td>0.147</td>
<td>1.0</td>
</tr>
<tr>
<td>2. Modified Program</td>
<td>0.1409</td>
<td>0.154</td>
<td>1.0</td>
</tr>
<tr>
<td>(a) New enthalpy computation, equation (46)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(b) Sutherland viscosity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Modified Program</td>
<td>0.1411</td>
<td>0.172</td>
<td>1.37</td>
</tr>
<tr>
<td>(a) New enthalpy computation, equation (46)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(b) New viscosity, equation (48)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
For these runs, conditions were chosen at which the modifications in viscosity and enthalpy computation would have their greatest effect. These conditions are the ones which yield a high degree of dissociation and ionization, equations (46) and (48), i.e. high speed and high freestream density. Therefore, an altitude was chosen (86 km) where freestream density is near the maximum for which the program will run (see General Results section). The table shows that the enthalpy and viscosity modifications had a significant effect on heat transfer rate and shock layer thickness. The heat transfer rate was increased 17 percent due to the combined effect of both modifications.

C. Comparison with Experimental Data

Very little experimental data exist for the low density, hypersonic, high stagnation enthalpy flow regime for which this computer program was designed. Therefore, we do not have the detailed comparison with experimental data which is desired to validate the present analysis. However, a limited amount of heat transfer and pressure data for spheres are available from an arc-jet facility at moderate stagnation enthalpy [15], and a larger body of stagnation heat transfer data exists for relatively low enthalpy, and hypersonic flow [16].

Figure 2 compares computed stagnation point heat transfer coefficients, \( C_H \), for a sphere with experimental data from References 15 and 16. The data in this figure represent several levels of stagnation enthalpy and, hence, several levels of real gas effects, so good agreement among all the data is not expected. The purpose here is to compare the computed results directly with each set of experimental data and to observe the trend in \( C_H \) with changing stagnation enthalpy. A best fit curve through the relatively low enthalpy data of Vidal and Wittliff [16] is shown by the solid line, and the square symbols give the computed values for the same flow conditions. Although the computer program was designed for real gas, chemically reacting flows, it can be run at the low enthalpy conditions of the Vidal and Wittliff data, in which case the computed dissociation levels are very low. The data are plotted as a function of the similarity parameter, \( K^2 \), used by Vidal and Wittliff, and defined as follows:

\[
K^2 = \frac{Re_\infty}{\gamma \infty \ M^2 \infty \ C^*}, \tag{62}
\]
Figure 2. Comparison of present theory with experimental data for stagnation point heating on a sphere.
where

\[ C^* = \frac{\mu^*}{\mu_\infty} \frac{\bar{T}_\infty}{\bar{T}^*} \]  \hspace{1cm} (63)

and

\[ \bar{T}^* = \frac{1}{2} \left( \bar{T}_{0\infty} + \bar{T}_w \right) \] \hspace{1cm} (64)

where

\[ \mu^* = \text{viscosity computed by Sutherland's formula using } \bar{T}^* \]

\[ \mu_\infty = \text{viscosity computed by Sutherland's formula using } \bar{T}_\infty . \]

The computed data do not agree with the mean of the Vidal and Wittliff data as well as we would like, but the computed data points fall within the scatter of the experimental points [16]. The computed values tend to overestimate \( C_H \) at rarefied conditions and underestimate it for denser flow. It is important to note that at the higher enthalpy cases, the wall catalysis can affect the value of \( C_H \) by a factor of 3 or more [4]. Hence, any comparison of experimental and calculated heating must be for similar wall catalysis.

The arc-jet data of Scott [15] are shown by the filled diamond symbols, and computed data for the same conditions are shown by the empty diamond symbols. The flow conditions for these tests are given in Table 2.

The freestream boundary conditions in the computer program were modified to match the dissociated arc-jet freestream. Also, the spheres in the arc-jet tests were coated with teflon to produce a noncatalytic wall and, therefore, the noncatalytic wall option in the computer program was used for comparison with these data points. The noncatalytic wall option was also used for the remainder of the computer data in this figure and the entire report unless otherwise noted.

The comparison of the computed data with Scott's experimental data is considered acceptable.
TABLE 2. ARC-JET FLOW FIELD PROPERTIES

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach number, $M_\infty$</td>
<td>10</td>
<td>8</td>
</tr>
<tr>
<td>Reynolds number, $Re_\infty$</td>
<td>380</td>
<td>553</td>
</tr>
<tr>
<td>Freestream speed, $\bar{V}_\infty$ (cm/sec)</td>
<td>423 000</td>
<td>412 000</td>
</tr>
<tr>
<td>Freestream temperature, $\bar{T}_\infty$ (K)</td>
<td>270</td>
<td>414</td>
</tr>
<tr>
<td>Freestream density, $\bar{\rho}_\infty$ (gm/cm³)</td>
<td>$3.28 \times 10^{-8}$</td>
<td>$6.41 \times 10^{-8}$</td>
</tr>
<tr>
<td>Wall temperature, $\bar{T}_w$ (K)</td>
<td>450</td>
<td>450</td>
</tr>
<tr>
<td>Radius of sphere, $r_b$ (cm)</td>
<td>5.08</td>
<td>5.08</td>
</tr>
<tr>
<td>Species mass fractions in freestream:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$N_2$</td>
<td>0.4138</td>
<td>0.6124</td>
</tr>
<tr>
<td>$O_2$</td>
<td>$0.6519 \times 10^{-5}$</td>
<td>$0.1084 \times 10^{-4}$</td>
</tr>
<tr>
<td>$N$</td>
<td>0.3514</td>
<td>0.1522</td>
</tr>
<tr>
<td>$O$</td>
<td>0.2348</td>
<td>0.2347</td>
</tr>
<tr>
<td>NO</td>
<td>$0.5380 \times 10^{-5}$</td>
<td>$0.3761 \times 10^{-4}$</td>
</tr>
<tr>
<td>$NO^+$</td>
<td>$0.2221 \times 10^{-5}$</td>
<td>$0.6849 \times 10^{-5}$</td>
</tr>
<tr>
<td>$e^-$</td>
<td>$0.3850 \times 10^{-10}$</td>
<td>$0.1187 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

Some high-enthalpy computed data, for which the dissociation and ionization levels are very high, are shown in Figure 2 by the circular symbols. These data points fall considerably below the lower enthalpy data at the continuum end of the flow regime (at large values of $K^2$) where there is a consistent trend of decreasing $C_H$ with increasing enthalpy for a given $K^2$. The parameter $K^2$ does not account for real gas effects and, therefore, should not be expected to correlate data with widely different enthalpy levels.
Acceptable comparisons have also been obtained with other theoretical predictions by Kumar and Jain [3] who used an analysis identical to the present one except for slip, enthalpy, and viscosity computations.

D. General Results

Figures 3 and 4 illustrate typical convergence behavior of the solutions with increasing number of iterations. Figure 3 shows the successive computed nondimensional temperature profiles, including the initial guess, along the stagnation streamline of a sphere with noncatalytic wall. The temperature profiles did not quite converge by the final iteration (2000), so it was necessary to make a rerun using the output of run No. 1 as input data for run No. 2. The figure illustrates that extremely accurate initial guesses are not generally required to achieve convergence; however, the more accurate the initial guess, the faster the solutions will converge. At very large Reynolds numbers, where gradients in flow properties are large, more accurate initial guesses are required to avoid divergence. Figure 4 shows the convergence behavior of wall heat transfer coefficient, \( C_H \), for the same run. The converged value of \( C_H \), obtained in run No. 2, is shown at the right margin.

Figure 5a gives the computed velocity components, and the pressure, temperature, and density profiles along the stagnation streamline of a sphere with noncatalytic wall at relatively high freestream Reynolds number (1315). Figure 5b gives the mass fraction profiles for the same run. This run is approaching the maximum Reynolds number for which the program will converge easily without extremely accurate input data or modifications to the program such as spacing the computation increments closer together. The meaning of the quantities in Figure 5a are given in equations (18) through (24); e.g. \( P_I \) is the pressure on the stagnation streamline, and \( P_2 \) gives the correction in pressure for small angles away from the stagnation streamline. A thick "shock wave" is indicated by the steep gradients in the region \( 1.06 < r < 1.12 \).

The same quantities presented in Figure 5 are plotted in Figure 6 for a smaller Reynolds number (185). Figure 6a reveals that all evidence of a shock wave has disappeared at this low Reynolds number. Comparison of Figures 5b and 6b shows that the degree of dissociation and ionization decreases drastically in lower density flow.

Figure 7 gives the flow profiles along the stagnation streamline of a sphere with fully catalytic wall at a medium Reynolds number (458). The Sutherland viscosity formula was used because this run was made before the
Figure 3. Convergence of temperature profiles for sphere with increasing number of iterations.
Figure 4. Typical convergence of stagnation point heat transfer coefficient for sphere with increasing number of iterations.
Figure 5. Flow profiles for sphere with noncatalytic wall at large Reynolds number \((Re_\infty = 1315)\).
Figure 5. (Concluded)

b. Mass fraction profiles.
HANSEN'S VISCOSITY
ALTITUDE = 96 km
\( \bar{r}_0 = 30.5 \text{ cm} \)
\( V_\infty = 793,000 \text{ cm/s} \)
\( \bar{\rho}_\infty = 0.1008 \times 10^{-8} \text{ gm/cm}^3 \)
\( \bar{T}_\infty = 198.45 \text{ K} \)
\( \bar{T}_W = 600 \text{ K} \)

a. Velocity and thermodynamic property profiles.

Figure 6. Flow profiles for sphere with noncatalytic wall at small Reynolds number (Re\(_\infty\) = 185).
b. Mass fraction profiles.

Figure 6. (Concluded)
a. Velocity and thermodynamic property profiles.

Figure 7. Flow profiles for sphere with fully catalytic wall ($Re_\infty = 458$).
b. Mass fraction profiles.

Figure 7. (Concluded)
viscosity modification to the program. The density profile gives a hint of a shock wave similar to that shown in Figure 5a. Comparison of Figures 5b, 6b, and 7b illustrate the difference in species mass fraction profiles between a noncatalytic wall and a fully catalytic wall. The species mass fractions approach their freestream values at the catalytic wall except for the ions NO\(^+\) and e\(^-\). The wall is assumed noncatalytic with respect to ion recombination in this program.

Figures 5 through 7 provide useful starting data for running the program at conditions near the ones in these figures.

Figure 8 compares temperature, density, and velocity profiles for a sphere and cylinder at the same flow conditions as in Figure 5. The profiles are remarkably similar. Therefore, the profiles for a sphere, Figures 5, 6, and 7, are adequate to use as starting data for the cylindrical option of the program.

The change in the stagnation line temperature profile with freestream density, or Re\(_\infty\), is illustrated in Figure 9. The peak value in nondimensional temperature decreases and the shock layer thickness increases with increasing altitude or decreasing density.

The freestream density and speed greatly affect the degree of dissociation of the air molecules and, hence, the viscosity of the gas mixture. Figure 10 gives the peak values from the viscosity and mass fraction profiles for N, O, and NO as a function of altitude for a fixed large value of freestream speed. As before, the freestream thermodynamic properties associated with altitude are obtained from Reference 14. Although the stagnation enthalpy is large, the figure shows that dissociation becomes negligible and viscosity approaches the Sutherland value at altitudes greater than approximately 100 km. This is due to the decreased reaction rates at the lower temperatures which occur in the shock layer at higher altitudes (Fig. 9). Figure 11 illustrates that dissociation and the viscosity ratio increase with increasing freestream speed at the fixed altitude of 96 km.

A parametric study was made to determine the effect of altitude (or density), freestream speed, and wall temperature on the stagnation point heat transfer coefficient, C\(_H\). Figure 12 gives C\(_H\) for a sphere and cylinder as a function of altitude with fixed freestream speed and wall temperature. Hansen's viscosity, equation (48), was used for the sphere, but Sutherland's viscosity was used for the cylinder because those runs were made before the program was modified to compute Hansen's viscosity. The figure shows a steady increase
Figure 8. Comparison of flow profiles for sphere and cylinder.
Figure 9. Temperature profiles at various Reynolds numbers for sphere.
Figure 10. Effect of variation in altitude on dissociation and viscosity in shock layer of sphere.
Figure 11. Effect of freestream speed on dissociation and viscosity in shock layer of sphere.
NONCATALYTIC WALL

\( \nabla_\infty = 793,000 \text{ cm/s} \)

\( \bar{T}_W = 600 \text{ K} \)

\( \bar{r}_b = 30.5 \text{ cm} \)

Figure 12. Stagnation point heat transfer coefficients for spheres and cylinders as a function of altitude.
in $C_H$ with increasing altitude. The theoretical free molecular value ($C_H = 1.0$) is exceeded for the sphere at approximately 106 km and for the cylinder at approximately 109 km. The curves continue to climb with increasing slope at higher altitudes. This unrealistic behavior for a fixed wall temperature might be attributed to a breakdown in the continuum approach (Navier-Stokes equations with slip boundary conditions) at extremely high altitudes and low densities. In particular, the assumption of a thin Knudsen layer, which is implicit in the present analysis, becomes invalid at very low densities. One must also consider the practicality of a specified $T_w$ in rarefied flow. This breakdown is gradual, and one cannot pinpoint a sharp boundary beyond which the program gives invalid results. However, the results should be treated with increasing skepticism, for this body size and flow conditions, at altitudes greater than approximately 104 km, or $Re_\infty < 40$.

An interesting feature of Figure 12 is the crossover of the curves for the sphere and cylinder. This crossover should not be attributed to the differences in viscosity computation because the effects of Hansen's viscosity (used for the sphere but not for the cylinder) is to increase $C_H$ at low altitudes but not to affect $C_H$ at high altitudes where dissociation is negligible. Therefore, if Hansen's viscosity were also used for the cylinder, the crossover of the two curves should be expected at a higher altitude. The explanation for this crossover is a result of the stronger merged shock layer effect on the sphere.

The variation of $C_H$ with freestream speed for a sphere at fixed altitude (96 km) and wall temperature (600 K) is shown in Figure 13. The effect of increasing freestream speed, or stagnation enthalpy, is to decrease $C_H$.

Figure 14 gives the variation in $C_H$ with wall temperature for a sphere at fixed altitude (96 km) and speed (793 000 cm/sec). An increase in wall temperature produces an increase in $C_H$.

The data in Figures 12 through 14 are replotted in Figure 15 as a function of $K^2$; the similarity parameter is given by equation (62). This parameter includes all the independent variables in Figures 12, 13, and 14, but the effect of freestream density is obviously dominant in determining the value of $K^2$ and $C_H$. The data were also plotted as a function of other similarity parameters (not shown), but $K^2$ correlated the data as well as, or better than, any of the other parameters. This is not the case if wall catalysis is varied. Therefore, $K^2$ was selected as the similarity parameter to use in presenting the remainder of the data.
HANSEN'S VISCOSITY
NONCATALYTIC WALL
ALT = 96 km
$\bar{r}_b = 30.5 \text{ cm}$
$\bar{T}_W = 600 \text{ K}$

Figure 13. Stagnation point heat transfer coefficient for sphere as function of freestream speed.
HANSENS'S VISCOSITY NONCATALYTIC WALL

$\bar{V}_\infty = 793 \, 000 \, \text{cm/s}$

$\text{ALT} = 96 \, \text{km}$

$\bar{r}_b = 30.5 \, \text{cm}$

$Re_\infty = 185$

Figure 14. Stagnation point heat transfer coefficient for sphere as function of wall temperature.
Figure 15. Stagnation point heat transfer coefficient for sphere as function of $K^2$. 

HANSEN'S VISCOSITY NONCATALYTIC WALL

$R_b = 30.5$ cm

ALTITUDE VARIATION
$V_{\infty}$ VARIATION
$T_W$ VARIATION
Figure 16 gives the nondimensional shock layer thickness, $n_{\infty}$, for spheres and cylinders as a function of $K^2$. The shock layer is thin at the continuum end (large $K^2$) of the flow regime and becomes very thick at highly rarefied conditions (small $K^2$).

Figure 17 presents the computed slip speed for a sphere and cylinder as a function of $K^2$. The slip speed is computed at the outer edge of the Knudsen layer, but it is applied at the wall in the outer flow solution, i.e., a thin Knudsen layer is assumed. This is a source of error at high altitudes where the Knudsen layer thickness becomes significant. The slip speed is greatly affected by variation in freestream speed and wall temperature. However, these effects are not correlated well by the parameter $K^2$ as shown for the sphere by the partially filled symbols. To estimate the slip speed for given conditions, one can extrapolate from the solid curves using the partially filled symbols as a guide in correcting for freestream speed and wall temperature. Once again it appears that the proper $T_w$ must be used for rarefied flow calculations. The decrease in slip speed with increasing altitude (decreasing $K^2$) at high altitude (small $K^2$) seems unrealistic and has been criticized. However, decreasing slip speed decreases the $C_H$ computed by this program. Since the computed $C_H$ is too large at high altitudes for a fixed $T_w$ (Figs. 12 and 15), the decrease in slip speed at high altitudes tends to compensate for the overprediction of $C_H$ and is, from a practical standpoint, a favorable phenomenon.

The temperature at the edge of the Knudsen layer is given as a function of $K^2$ in Figure 18. This temperature also depends strongly on freestream speed and wall temperature.

The information in Figures 15 through 18 is useful as input data in running the computer program (Appendix A).

An example of the practical use of this computer program is given in Figure 19. Stagnation point heating rates for the spherical nose of the Space Shuttle External Tank are given as a function of trajectory time. The solid curve is the heating rate predicted by the MSFC Thermal Environment Branch (ED33) and is based on theoretical continuum methods at low altitudes and experimental data at high altitudes. The filled diamond symbols were computed using the present program. The trajectory time interval from approximately 275 to 475 sec corresponds to an altitude interval which is too high for this program, i.e., the predicted values of $C_H$ were unrealistically large. For a
Figure 16. Shock layer thickness for sphere and cylinder.
Figure 17. Slip speed at body surface for sphere and cylinder.
Figure 18. Temperature of air at wall for sphere and cylinder.
Figure 19. Space Shuttle external tank stagnation point heating rate.
body of this size \( f_b = 30.5 \text{ cm} \), the altitude interval for which this program is applicable is approximately 86 to 105 km. For this altitude interval, the predicted values from this program agree quite well with the predictions from experimental data for a known \( T_w \).
APPENDIX A. COMPUTER PROGRAM
APPENDIX A. COMPUTER PROGRAM

General Information

The computer program is written in Fortran IV language, and it is run on the Univac 1108 computer at MSFC. As currently written, the program is limited to a maximum of 2000 iterations. If convergence is not achieved in 2000 iterations, the program is rerun using the output from the first run as starting data for the second run.

The program has three options:

(1) Body: sphere or two-dimensional circular cylinder
(2) Wall catalyticity: noncatalytic wall or fully catalytic wall
(3) Viscosity: Sutherland or Hansen's high temperature model.

The choices made in options (1) and (2) make very little difference in the computer time used. However, the Hansen viscosity option takes significantly more computer time than the Sutherland option; e.g., if the full 2000 iterations are used, the Sutherland option takes approximately 8 min and the Hansen option takes about 10 min.

Program Input

The quantities needed for input to the program are defined and their functions described as follows:

<table>
<thead>
<tr>
<th>Computer Program Variable</th>
<th>Symbol Used in Report</th>
<th>Dimensions</th>
<th>Description</th>
<th>Suggested Source or Range of Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>EFFR1</td>
<td>n∞</td>
<td>Dimensionless</td>
<td>Initial guess for nondimensional shock layer thickness</td>
<td>Figure 16</td>
</tr>
<tr>
<td>TOL</td>
<td></td>
<td>Dimensionless</td>
<td>Computation is stopped when ( C_H ) converges within a prescribed tolerance. If ( \left</td>
<td>\frac{C_H}{C_{H_{N-1}}} \right</td>
</tr>
<tr>
<td>EPSI</td>
<td></td>
<td>Dimensionless</td>
<td>Maximum change allowed in all computed dimensional quantities from one iteration to the next</td>
<td>0.001 - 0.005</td>
</tr>
<tr>
<td>Computer Program Variable</td>
<td>Symbol Used in Report</td>
<td>Dimensions</td>
<td>Description</td>
<td>Suggested Source or Range of Values</td>
</tr>
<tr>
<td>---------------------------</td>
<td>-----------------------</td>
<td>------------</td>
<td>-------------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td>ALT</td>
<td>km</td>
<td>Altitude corresponding to the freestream thermodynamic properties (used for identification only)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RADB</td>
<td>cm</td>
<td>Radius of body</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UFS</td>
<td>cm/s</td>
<td>Freestream speed</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TFS</td>
<td>K</td>
<td>Freestream temperature</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TWK</td>
<td>K</td>
<td>Temperature of body surface</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ROFS</td>
<td>gm/cm³</td>
<td>Freestream density</td>
<td></td>
<td></td>
</tr>
<tr>
<td>U(1)</td>
<td>Dimensionless</td>
<td>Initial guess for ( \frac{u}{u_W} \text{sin}\theta )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T(1)</td>
<td>Dimensionless</td>
<td>Initial guess for nondimensional temperature of gas at outer edge of Knudsen layer</td>
<td></td>
<td></td>
</tr>
<tr>
<td>U(1)</td>
<td>Dimensionless</td>
<td>Initial guess for ( u_1 ) (see equation 19) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>V(1)</td>
<td>Dimensionless</td>
<td>Initial guess for ( v_1 ) (see equation 19) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T(1)</td>
<td>Dimensionless</td>
<td>Initial guess for ( T_1 ) (see equation 20) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RO(1)</td>
<td>Dimensionless</td>
<td>Initial guess for ( \rho_1 ) (see equation 21) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P2(I)</td>
<td>Dimensionless</td>
<td>Initial guess for ( P_2 ) (see equation 22) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO2(I)</td>
<td>Dimensionless</td>
<td>Initial guess for mass fraction of ( O_2 ) at location ( I = 2, 3, \ldots, 50 )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 17

Figure 18

Figures 5-7

Figures 5-7

Figures 5-7

Figures 5-7

Figures 5-7

Figures 5-7

Figures 5-7
<table>
<thead>
<tr>
<th>Computer Program Variable</th>
<th>Symbol Used in Report</th>
<th>Dimensions</th>
<th>Description</th>
<th>Suggested Source or Range of Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNO1(I)</td>
<td>Y&lt;sub&gt;NO&lt;/sub&gt;&lt;sup&gt;+&lt;/sup&gt;</td>
<td>Dimensionless</td>
<td>Initial guess for mass fraction of NO&lt;sup&gt;+&lt;/sup&gt; at location I (I = 2, 3, ..., 50)</td>
<td>Figures 5-7</td>
</tr>
<tr>
<td>CNO(I)</td>
<td>Y&lt;sub&gt;NO&lt;/sub&gt;</td>
<td>Dimensionless</td>
<td>Initial guess for mass fraction of NO at location I (I = 2, 3, ..., 50)</td>
<td>Figures 5-7</td>
</tr>
<tr>
<td>CN(I)</td>
<td>Y&lt;sub&gt;N&lt;/sub&gt;</td>
<td>Dimensionless</td>
<td>Initial guess for mass fraction of N at location I (I = 2, 3, ..., 50)</td>
<td>Figures 5-7</td>
</tr>
<tr>
<td>CO(I)</td>
<td>Y&lt;sub&gt;O&lt;/sub&gt;</td>
<td>Dimensionless</td>
<td>Initial guess for mass fraction of O at location I (I = 2, 3, ..., 50)</td>
<td>Figures 5-7</td>
</tr>
</tbody>
</table>

The quantities U(I) through CO(I) must be input for each of the 49 equally-spaced points in the shock layer along the stagnation streamline starting with I = 2 near the wall and ending with I = 50 near the freestream (see Fig. A-1). The wall (I = 1) and freestream (I = 51) boundary conditions are given by the quantities UFS through T(1).

The quantities U(I) through CO(I) must be input for each of the 49 equally-spaced points in the shock layer along the stagnation streamline starting with I = 2 near the wall and ending with I = 50 near the freestream (see Fig. A-1). The wall (I = 1) and freestream (I = 51) boundary conditions are given by the quantities UFS through T(1).

The format for the input data is as follows:

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Variable Name(s)</th>
<th>Location and Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12A6</td>
<td>AB1, ..., AB/2</td>
<td>Columns 1-72 contain a comment for project identification</td>
</tr>
<tr>
<td>2</td>
<td>3F10.0</td>
<td>XBOD</td>
<td>Columns 1-10 contain the body option (sphere = 1.0, cylinder = 2.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>XCAT</td>
<td>Columns 11-20 contain the wall catalyticity option (noncatalytic wall = 1.0, fully catalytic wall)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>XVIS</td>
<td>Columns 21-30 contain the viscosity option (Sutherland viscosity = 1.0, Hansen viscosity = 2.0)</td>
</tr>
<tr>
<td>3</td>
<td>2F10.0</td>
<td>CASE</td>
<td>Columns 1-10 contain the run number. This identification is useful to distinguish between runs whenever a rerun is necessary</td>
</tr>
<tr>
<td>Card</td>
<td>Format</td>
<td>Variable Name(s)</td>
<td>Location and Description</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>-----------------</td>
<td>------------------------</td>
</tr>
<tr>
<td>4</td>
<td>2F10.0</td>
<td>EFFR1</td>
<td>Columns 11-20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TOL</td>
<td>Columns 1-10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>EPSI</td>
<td>Columns 11-20</td>
</tr>
<tr>
<td>5</td>
<td>5F10.0</td>
<td>ALT</td>
<td>Columns 1-10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RADB</td>
<td>Columns 11-20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>UFS</td>
<td>Columns 21-30</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TFS</td>
<td>Columns 31-40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWK</td>
<td>Columns 41-50</td>
</tr>
<tr>
<td>6</td>
<td>E13.8</td>
<td>ROFS</td>
<td>Columns 1-13</td>
</tr>
<tr>
<td>7</td>
<td>2F10.0</td>
<td>U(1)</td>
<td>Columns 1-10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>T(1)</td>
<td>Columns 11-20</td>
</tr>
<tr>
<td>8-56</td>
<td>5E16.9</td>
<td>U(1)</td>
<td>Columns 1-16</td>
</tr>
<tr>
<td></td>
<td></td>
<td>V(1)</td>
<td>Columns 17-32</td>
</tr>
<tr>
<td></td>
<td></td>
<td>T(1)</td>
<td>Columns 33-48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RO(I)</td>
<td>Columns 49-64</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P2(I)</td>
<td>Columns 65-80</td>
</tr>
<tr>
<td>57-105</td>
<td>5E16.9</td>
<td>CO2(I)</td>
<td>Columns 1-16</td>
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<td></td>
<td></td>
<td>CNOI(i)</td>
<td>Columns 17-32</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CNO(I)</td>
<td>Columns 33-48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CN(I)</td>
<td>Columns 49-64</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO(I)</td>
<td>Columns 65-80</td>
</tr>
</tbody>
</table>
PROGRAM OUTPUT

The program printout is described in this section. Figure 5 of the text was obtained from this printout. Explanation of the printout follows.

Title Page

Options used — The options which were selected for body, wall catalyticity, and viscosity are printed out here.

Input data — The input data are printed out for record.

Computed freestream data — Some freestream quantities which are used for nondimensionalizing and for computation of various similarity parameters are printed here. The equations used are as follows:

\[
V_{\text{SOUND}} = \sqrt{\frac{\gamma R T_\infty}{\mu}} \quad [\text{cm/sec}] \quad , \quad (A-1)
\]

where

\[
\gamma = 1.4 \\
\bar{R} = 2.8708 \times 10^6 \text{ cm}^2/\text{sec}^2\text{K} \\
\mu_\infty = \frac{\text{UFS}}{V_{\text{SOUND}}} \quad (A-2)
\]

\[
\bar{T}_0 = \text{STAGFS} = \bar{T}_\infty \left( 1 + \frac{\gamma - 1}{2} \frac{M_\infty^2}{\mu_\infty} \right) \quad [^\circ\text{K}] \quad (A-3)
\]

\[
\mu_\infty = \text{RTFS} = \frac{1.458 \times 10^{-5} \bar{T}_\infty}{\bar{T}_\infty + 110.4} \quad [\text{gm/cm}\cdot\text{sec}] \quad (A-4)
\]

\[
\mu_0 = \text{RTSTAG} = \frac{1.458 \times 10^{-5} \bar{T}_0}{\bar{T}_0 + 110.4} \quad [\text{gm/cm}\cdot\text{sec}] \quad . \quad (A-5)
\]
It is recognized that the stagnation temperature, equation (A-3), has little physical meaning at the high stagnation enthalpies for which this computer program is intended. This is because equation (A-3) is based on the assumption of constant specific heat for temperatures up to $T_{0\infty}$; the assumption of constant specific heat is violated at moderate temperatures. However, $T_{0\infty}$ is used only for nondimensionalizing and for computing $\mu_{0\infty}$. It does not influence the computation of the flow field in any way. Likewise, $\mu_{0\infty}$ is a fictitious viscosity because $T_{0\infty}$ is fictitious and also because the Sutherland formula is not applicable at high temperatures.

Similarity Parameters — Some similarity parameters are printed out here. Several of these have been used, with some success, in correlating hypersonic or low density data. The similarity parameters are defined as follows:

\[ Re_{\infty} = REYF = \frac{\dot{\rho}_{\infty} V_\infty r_b}{\mu_{\infty}} \quad (A-6) \]

\[ Re_{0\infty} = REYN = \frac{\dot{\rho}_{\infty} V_\infty r_b}{\mu_{0\infty}} \quad (A-7) \]

\[ Re_w = REWALL = \frac{\dot{\rho}_{\infty} V_\infty r_b}{\mu_w} \quad (A-8) \]

where $\mu_w$ is computed by the Sutherland formula using $T_w$.

\[ K_{n_{\infty}} = XKNFS = \frac{\lambda_{\infty}}{r_b} \quad (A-9) \]
\[ \bar{V} = \text{VBAR} = M_\infty \sqrt{\frac{C_\infty}{\text{Re}_\infty}} , \]  

(A-10)

where

\[ C_\infty = \frac{\bar{\mu}_w}{\bar{\mu}_\infty} \frac{\bar{T}_\infty}{\bar{T}_w} . \]

(A-11)

\[ K^2 = \text{XKSQ} = \frac{\text{Re}_\infty}{\gamma_\infty M_\infty^2 C_*} , \]

where

\[ C_* = \frac{\bar{\mu}_*}{\bar{\mu}_\infty} \frac{\bar{T}_\infty}{\bar{T}_*} , \]

and

\[ T_* = \frac{1}{2} (\bar{T}_0 + \bar{T}_w) \]

\[ \bar{\mu}_* = \text{Sutherland viscosity computed at } \bar{T}_* . \]

The similarity parameter \( \phi \) is given as the final item in the printout. It is placed in this location because it uses the computed enthalpy at the wall. This parameter was suggested by Potter (Rarefied Gas Dynamics, Supplement 5, Vol. I, 1969).

\[ \phi = \text{PHI} = \text{Re}_w \left( \frac{2h}{\bar{W}} \right)^{0.6} \left( \frac{\bar{V}_\infty}{\bar{V}} \right) , \]  

(A-12)
Data Pages

A set of computed data is printed out after every 200 iterations. Each set of data consists of three pages.

1. **First Page.** The computed shock layer thickness (EFFR) and wall heat transfer coefficient \( C_H \) are printed at the top of the page after every 50 iterations. The control factors which are used to update the computed quantities to obtain input variables for the next iteration are also printed here.

The columns on this page give nondimensional values of (1) radial position from the center of the body to the equally-spaced points at which the independent variables are computed, (2) the velocity component \( u_1 \) [see equation (18)], (3) the velocity component \( v_1 \) [see equation (19)], (4) specific enthalpy, (5) temperature, (6) viscosity ratio, local ratio of Hansen viscosity to Sutherland viscosity, (7) pressure \( P_1 \) [see equation (22)], (8) pressure correction \( P_2 \) [see equation (22)], and (9) density.

Note that VFS is the same as UFS elsewhere in the program. It is the freestream speed \( \bar{V}_\infty \).

2. **Second Page.** This page gives the reaction rates for each of the seven species.

3. **Third Page.** This page gives the mass fractions of the chemical species which compose the air. Note that mass fraction was denoted by "Y" in the text rather than by "C." The electron number density is also given.

When \( C_H \) converges within the prescribed tolerance, or when the iterations reach 2000, the iterations are stopped and the final data set is printed out. At this point a set of 98 cards is punched to record the velocity and thermodynamic data given on page 1 and the mass fraction data on page 3 of the data printout. This set of cards can then be used as starting data for a new run.

To determine whether or not the program has converged sufficiently and whether the results are reasonable, the following checks are suggested.

(1) Check EFFR for convergence

(2) Check \( C_H \) for convergence
(3) Check the slip conditions for convergence, i.e. compare U₁ and T at RAD/RADB = 1.0 for the last few sets of data

(4) Scan the velocity component and thermodynamic property columns to determine if the profiles are smooth and the values are reasonable

(5) Scan the mass fraction columns to check for reasonable behavior. Particularly check the N₂ column near the wall to determine if these mass fractions exceed the freestream value.

SOME DIFFICULTIES ENCOUNTERED IN RUNNING PROGRAM

The program generally runs without much difficulty if the starting data are within reasonable bounds; however, problems do occur, and some of the most common problems are discussed as follows.

1. Failure of EFFR to Converge. The shock layer thickness, EFFR, usually is the first quantity to converge; however, it sometimes diverges. The most common cause of this is using starting data from a run with a much different stagnation enthalpy, or \( T_{om} \), from the case being run. This causes a discontinuity in the nondimensional temperature profile between the points \( I = 50 \) and \( I = 51 \) because the point \( I = 50 \) comes from the starting data from a previous run and point \( I = 51 \) is the freestream boundary condition. The decision on whether to decrease, increase, or not change EFFR is made on the basis of the temperature gradient near the freestream (see Appendix B). Therefore, if a sizable discontinuity in temperature exists at this location, EFFR will diverge.

One solution to this problem is to modify the last few input cards to make a smooth transition in the temperature profile to the freestream temperature. Probably a better solution would be to change the nondimensionalizing temperature from \( T_{0\infty} \) to \( T_{\infty} \). This would guarantee a smooth transition, in the starting data, to the freestream temperature. To prevent divergence of EFFR, the program has been modified to restrict EFFR within the range.
\[ \frac{1}{2} \text{EFFR}_1 \leq \text{EFFR} \leq \frac{3}{2} \text{EFFR}_1. \]

If EFFR\(_1\) is not guessed closely enough, this restriction will necessitate a rerun using a different EFFR\(_1\).

2. **Unrealistic Chemical Composition.** If the species mass fractions in the starting data are greatly different from the true values for the case being run, unrealistic computed mass fractions can result. This can lead to unrealistic computed values for all other quantities. For example, this might occur for a rather low speed, high density case in which dissociation should be negligible (Fig. 11). However, since starting data from a low speed, high density run were not available, data were used from a high speed, high density run in which the degree of dissociation was high. The program could not handle the grossly incorrect starting data, and the computed results became more and more unrealistic from one iteration to the next. The unrealistic data included mass fractions for \(N_2\) much larger than the freestream value, negative \(C_H\) (heat transferred from the body to the gas) and a monotonically increasing EFFR beyond reasonable bounds (Fig. 16). Note that \(C_H\) was called "STANC" in the older printout.

**SOME SUGGESTIONS FOR RUNNING PROGRAM**

To minimize the previously discussed problems and to facilitate operation of the program, the following suggestions on input data are made.

1. **EFFR\(_1\), U(1), T(1), and TOL.** Figures 16, 17, and 18 can be used for obtaining initial guesses for EFFR\(_1\), U(1), and T(1), respectively. The value for TOL probably should be set smaller than the desired tolerance on \(C_H\) to assure that the other quantities converge also. A value of 0.00001 for TOL was used in most of the runs made for this report.

2. **Velocity, Thermodynamic Property, and Mass Fraction Profiles.** For best results, the starting data profiles for the quantities U(I) through CO(I) should be obtained from a run which matches the required freestream conditions of the new run as closely as possible. Close matching is especially important at low altitude, high density conditions for which gradients in the flow properties are large. The question arises as to what constitutes a
sufficiently close "match" and which matching, or similarity, parameter should be used. If every freestream and body condition is matched fairly closely, it is unnecessary to use a similarity parameter. From experience, it is found that, for a given body, changes in freestream density, \( \bar{\rho}_\infty \), and speed, \( \bar{V}_\infty \), in that order, have the greatest effect on the outcome of the run. Therefore, for bodies of the same size, one should try to match \( \bar{\rho}_\infty \) and \( \bar{V}_\infty \). A good rule of thumb is that \( \bar{\rho}_\infty \) for the new run should not differ from \( \bar{\rho}_\infty \) for the starting data run by more than the equivalent of 3 km altitude in the standard atmosphere. Near the low altitude extreme of the program's capability, this difference should not be more than approximately 1 km. A difference in \( \bar{V}_\infty \) of approximately 2000 m/sec can usually be tolerated. For bodies of greatly different size, one should probably use a similarity parameter, such as \( K^2 \), to match starting data to the new run.

Figures 5, 6, and 7 can be used for starting data. If the desired freestream properties for the new run are farther removed from those of Figures 5, 6, and 7 than the previously suggested increments, it is advisable to reach the desired conditions in two or more runs. If severe difficulties like those previously discussed are encountered, it is probably best to go back to a "good," or converged, set of starting data and use smaller increments in freestream properties rather than to use the output of the "bad" run as starting data for a rerun. If the program is used frequently, a library of starting data card sets can be built up to cover the range of possible freestream conditions for which the program is applicable.

3. Hansen-Sutherland Viscosity Option. If the computed ratio of Hansen's viscosity to Sutherland's viscosity is approximately 1.0 for a given set of freestream conditions, one can use the Sutherland viscosity option for nearby freestream conditions to reduce computer time.
Figure A-1. Location of computation points.
APPENDIX B. LISTING OF PROGRAM
Results of solving the Navier–Stokes equations for chemically nonequilibrium, merged stagnation shock layers on spheres and two-dimensional cylinders are presented. The effects of wall catalysis and slip are also examined. The thin shock layer assumption is not made, and the thick viscous shock is allowed to develop within the computational domain. The results show good comparison with existing data. Due to the more pronounced merging of shock layer and boundary layer for the sphere, the heating rates for spheres become higher than those for cylinders as the altitude is increased.
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