A new parabolized Navier-Stokes code for chemically reacting flow fields

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A new parabolized Navier-Stokes code for chemically reacting flow fields

Prabhu, Dinesh Kumble, Ph.D.

Iowa State University, 1987
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A new parabolized Navier-Stokes code for chemically reacting flow fields

by

Dinesh Kumble Prabhu

A Dissertation Submitted to the Graduate Faculty in Partial Fulfillment of the Requirements for the Degree of DOCTOR OF PHILOSOPHY
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NOMENCLATURE

\( A^* \) : reference area, \((m^2)\)

\( a_f \) : frozen speed of sound

\( C_d \) : total drag coefficient

\( C_f \) : skin-friction coefficient

\( C_h \) : heat transfer coefficient

\( C_p \) : pressure coefficient

\( C_{pf} \) : frozen specific heat of the mixture

\( c_s \) : mass fraction of species \( s \)

\( D \) : binary diffusion coefficient

\( h \) : specific static enthalpy

\( H \) : specific total enthalpy of the mixture

\( h^0_s \) : enthalpy of formation of species \( s \)

\( J \) : Jacobian of the coordinate transformation

\( k_{b,l} \) : backward reaction rate constant for the \( l \)th reaction

\( k_{f,l} \) : forward reaction rate constant for the \( l \)th reaction

\( L^* \) : reference length, \((m)\)

\( \mathcal{L}e \) : binary Lewis number

\( m^x, m^y, m^z \) : Cartesian components of the diffusion mass flux vector

\( m \) : number of reactions

\( M_f \) : frozen Mach number

\( M \) : molecular mass

\( n \) : number of species

\( N_A^- \) : Avogadro number, \(6.022169 \times 10^{20}\ \(kmol^{-1}\))
\( N_e^* \) \quad \text{electron number density,} \ (m^{-3})

\( n_t \) \quad \text{number of reactants (including catalytic third bodies)}

\( NJ \) \quad \text{number of grid points in the meridional direction}

\( NK \) \quad \text{number of grid points in the normal direction}

\( p \) \quad \text{static pressure of the mixture}

\( Pr_f \) \quad \text{frozen Prandtl number}

\( q_x, q_y, q_z \) \quad \text{Cartesian components of the heat flux vector}

\( R^* \) \quad \text{universal gas constant,} \ 8314.34 \ J/(kmol\cdot K)

\( Re \) \quad \text{Reynolds number based on} \ L^*

\( St \) \quad \text{Stanton number}

\( T \) \quad \text{static temperature of the mixture}

\( u, v, w \) \quad \text{Cartesian components of the mass-averaged velocity}

\( V \) \quad \text{magnitude of the mass-averaged velocity}

\( \dot{w}_s \) \quad \text{mass production rate of species} \ s

\( X_s \) \quad \text{mole fraction of species} \ s

\( x, y, z \) \quad \text{Cartesian coordinates (physical space)}

\( Z_{r,s} \) \quad \text{third body efficiency (relative to argon) of the} \ r\text{th catalytic body}

\( \alpha \) \quad \text{angle of attack}

\( \beta \) \quad \text{grid stretching parameter}

\( \gamma_s \) \quad \text{mole-mass ratio of species} \ s

\( \Delta \xi, \Delta \eta, \Delta \zeta \) \quad \text{mesh spacing in computational space}

\( \theta \) \quad \text{wedge or cone half angle}

\( \kappa \) \quad \text{thermal conductivity}

\( \mu \) \quad \text{molecular viscosity}

\( \xi, \eta, \varsigma \) \quad \text{generalized computational coordinates}
\( \rho \): mass density

\( \sigma \): safety factor

\( \tau \): shear stress

\( \omega \): streamwise pressure gradient parameter

Subscripts

\( i, j, k \): finite-difference indices

\( \text{ref} \): reference condition

\( r, s \): indices denoting species

\( w \): wall

\( x, y, z \): partial derivative with respect to \( x, y, z \)

\( \xi, \eta, \zeta \): partial derivative with respect to \( \xi, \eta, \zeta \)

\( \infty \): freestream

Superscripts

\( * \): dimensional quantity

\( c \): chemical quantity

\( i \): inviscid quantity

\( T \): transpose

\( v \): viscous quantity

\( x, y, z \): Cartesian components

\( \xi, \eta, \zeta \): transformed components
CHAPTER 1. INTRODUCTION

The recently proposed space transportation systems [1], [2] have sparked a renewed interest in hypersonic aerothermodynamics. The high-temperature shock layers around these vehicles will have many complex relaxation phenomena [3] such as vibrational excitation, chemical reactions, ionization, etc., taking place within them. Further, these relaxation processes are likely to be far from equilibrium at the high operational altitudes of the vehicles. At present, simulation of such finite-rate processes in ground-based experimental facilities is difficult. Hence, numerical simulation is necessary to predict the aerothermodynamic environments around these vehicles. The numerical simulation of complete thermochemical nonequilibrium has been successfully accomplished by Park [4]–[7] for one-dimensional flows. The extension of this analysis to higher dimensional flows is quite complicated and requires further research. However, as a first step, the problem can be simplified by assuming the flow field to be in thermal equilibrium but not in chemical equilibrium. The numerical simulation of viscous, chemically reacting, external flows around three-dimensional configurations is the focus of attention of several investigations today.

The numerical methods currently employed fall into two main categories, (i) time-marching methods and (ii) space-marching methods. In the time-marching methods [8]–[13], time-asymptotic solutions to the Navier-Stokes equations are computed. These methods are accurate but require a substantial amount of computer time. Space-marching methods, on the other hand, require much less computer time and provide accurate solutions in cases where they are applicable. In the latter category, some investigators [14]–[18] have analyzed inviscid chemical nonequilibrium
flow fields around complex geometries such as the Space Shuttle Orbiter. In order to account for viscous effects, the inviscid solutions have been coupled with matching boundary-layer analyses as described in Ref. 19. The success of Blottner [20], [21] in computing viscous reacting flows using boundary-layer methods has led to the development of a versatile reacting boundary-layer code [22]. The biggest drawback with the boundary-layer methods is the specification of edge conditions which can be quite difficult especially in the presence of entropy swallowing. In a seminal effort, Davis [23] developed a new set of equations called viscous shock-layer (VSL) equations. These equations are uniformly valid in the viscous and inviscid regions and thus overcome the drawbacks of the boundary-layer methods. Indeed, the VSL equations have been widely used [24]–[29] to compute three-dimensional, viscous, chemically reacting flow fields. The VSL equations are parabolic in both the streamwise and crossflow directions and therefore, they will fail in the presence of crossflow separation. Crossflow separation is routinely encountered on the leesides of vehicles at angle of attack. This deficiency is overcome through the use of the parabolized Navier-Stokes (PNS) equations [30]. These equations are also uniformly valid in the shock layer and have been, until recently, used for ideal and equilibrium gas flowfields. Bhutta et al. [31] were one of the first to use the PNS equations to compute chemical nonequilibrium flow fields. They solved the chemistry and gas dynamics separately and used an iterative approach to couple the two. This uncoupled iterative approach requires a few coupling parameters to bridge the gas dynamic and species equation sets. This task can become very difficult especially when the chemistry can have a strong influence on the flow and for thermochemical nonequilibrium situations. Therefore, direct coupling of gas dynamics and chemistry is the method of choice. The coupled approach leads to larger equation sets.
but this does not pose a problem due to the availability of supercomputers with large central core memories.

The aim of this study is to describe in detail the development of two new PNS codes for hypersonic chemically reacting flow fields. The study is divided into two parts. In the first part, the feasibility of the coupled approach is studied. Toward this end, a simple two-dimensional/axisymmetric PNS code is developed. The coupled set of gas dynamic and species conservation equations is solved using a finite-difference algorithm. The code is then used to compute hypersonic laminar flow of air consisting of five species \((O_2, O, N_2, N, NO)\) around wedges and cones. The results of these computations are shown to be in excellent agreement with those of reacting boundary-layer calculations [22]. Having established the feasibility of the coupled approach, a three-dimensional PNS code for chemical nonequilibrium flow fields is developed in the second part of this study. Again, the coupled set of gas dynamic and species equations is solved using an implicit, noniterative, approximately-factored, finite-difference method. The species set is enlarged to include ionized nitric oxide \((NO^+)\) and electrons \((e^-)\). The code is used to compute a number of chemically reacting flow fields around cones at angles of attack. The results of the computations are compared with those of a reacting boundary-layer code [22] and shown to be in excellent agreement.

It must be mentioned here that the present formulation of the problem differs from previous viscous formulations in the form of the energy equation used. Since the gases that constitute the reacting mixture are thermally perfect, the energy equation is usually written in terms of the mixture temperature. While such a formulation leads to the easier evaluation of thermodynamic and transport properties, it results in unwieldy source terms being added to the energy equation along with
a loss of the conservation-law form. In this study, the energy equation is written in terms of the total enthalpy of the mixture. Thus, the conservation-law form is retained. The mixture temperature is determined iteratively using the efficient Newton-Raphson method. This quadratically convergent method adds very little computing time.
CHAPTER 2. GOVERNING EQUATIONS

Navier-Stokes Equations

The equations governing the steady, three-dimensional laminar flow of a reacting mixture of gases have been obtained from the equations in Ref. 32 by (i) neglecting the time-derivative terms, (ii) assuming the flow to be in thermal equilibrium, (iii) neglecting radiation, and by (iv) assuming mass diffusion to be binary and due to concentration gradients only. These equations can be written in nondimensional, strong conservation-law form in Cartesian coordinates for an n-component system as:

\[ E'_x + F'_y + G'_z = \frac{1}{Re} \left( E^v_x + F^v_y + G^v_z \right) + W^c \]  \hspace{1cm} (1)

The \((n + 4)\)-component vector of conservation variables \(Q\) is chosen as

\[ Q = \{ \rho, \rho u, \rho v, \rho w, \rho H, \rho c_1, \rho c_2, \ldots, \rho c_{n-1} \}^T \]  \hspace{1cm} (2)

For this choice of dependent variables, the \((n + 4)\)-component inviscid flux vectors, \(E^i, F^i,\) and \(G^i\) are:

\[ E^i = \{ \rho u, \rho u^2 + p, \rho uv, \rho uw, \rho vH, \rho u c_1, \rho u c_2, \ldots, \rho u c_{n-1} \}^T \]

\[ F^i = \{ \rho v, \rho uv, \rho v^2 + p, \rho vw, \rho vH, \rho v c_1, \rho v c_2, \ldots, \rho v c_{n-1} \}^T \]

\[ G^i = \{ \rho w, \rho uw, \rho vw, \rho w^2 + p, \rho wH, \rho w c_1, \rho w c_2, \ldots, \rho w c_{n-1} \}^T \]

and the \((n + 4)\)-component viscous flux vectors \(E^v, F^v,\) and \(G^v\) are:

\[ E^v = \{ 0, \tau_{xx}, \tau_{xy}, \tau_{xz}, u \tau_{xx} + \tau_{xy} + \tau_{xz} - q, m_1, m_2, \ldots, m_{n-1} \}^T \]
\[ F^v = \{0, \tau_{xz}, \tau_{xy}, \tau_{yz}, u_x v_x + w_x v_y - q_x, m_1^y, m_2^y, \ldots, m_{n-1}^y \}^T \]

\[ G^v = \{0, \tau_{zx}, \tau_{zy}, \tau_{xy}, u_x v_x + w_x v_y - q_x, m_1^x, m_2^x, \ldots, m_{n-1}^x \}^T \]

where the components of the shear stress tensor, the heat flux vector and the diffusion mass flux vector are

\[
\begin{align*}
\tau_{xx} &= \frac{2}{3} \mu (2u_x - v_y - w_z) \\
\tau_{yx} &= \frac{2}{3} \mu (-u_x + 2v_y - w_z) \\
\tau_{zx} &= \frac{2}{3} \mu (-u_x - v_y + 2w_z) \\
\tau_{xy} &= \mu (u_y + v_x) \\
\tau_{yz} &= \mu (u_z + w_x) \\
\tau_{yx} &= \mu (v_y + w_x)
\end{align*}
\]

\[
\begin{align*}
q_x &= \beta_2 \kappa T_x + \sum_{s=1}^{n-1} (h_s - h_n) m_s^x \\
q_y &= \beta_2 \kappa T_y + \sum_{s=1}^{n-1} (h_s - h_n) m_s^y \\
q_z &= \beta_2 \kappa T_z + \sum_{s=1}^{n-1} (h_s - h_n) m_s^z
\end{align*}
\]

\[
\begin{align*}
m_x^s &= \beta_3 \rho D(c_s) x \\
m_y^s &= \beta_3 \rho D(c_s) y \\
m_z^s &= \beta_3 \rho D(c_s) z
\end{align*}
\]

The chemical source vector \( W^c \) is

\[ W^c = \{0, 0, 0, 0, \dot{w}_1, \dot{w}_2, \ldots, \dot{w}_s, \ldots, \dot{w}_{n-1} \}^T \]

where \( \dot{w}_s \) is the mass production or depletion rate of species \( s \). The mass production rate depends on the temperature, density and mass concentration of the reactants constituting the mixture and the expression for this rate is derived in Appendix A.

Note that the vector of dependent variables contains both the fluid dynamic and chemical variables and that only \((n - 1)\) of the \( n \) species continuity equations are required because the mass fractions sum to unity. Thus, the \( n \)th species
continuity equation is replaced by the following algebraic equation

\[ c_n = 1 - \sum_{s=1}^{n-1} c_s \]  

(3)

In addition to the above equations, the following equations are also used

\[ p = \frac{\beta_1 \rho T}{M} \]  

(4)

\[ H = h + \frac{1}{2}(u^2 + v^2 + w^2) \]  

(5)

\[ M = \left( \sum_{s=1}^{n} \frac{c_s}{M_s} \right)^{-1} \]  

(6)

where Eq. 4 is the equation of state for perfect gases, Eq. 5 is the definition of the mixture total enthalpy and Eq. 6 is the definition of the mixture molecular mass.

The following nondimensionalization has been employed in the present formulation

\[ x, y, z = \frac{x^*, y^*, z^*}{L^*} \quad p = \frac{p^*}{\rho_{\infty}^* V_{\infty}^2} \quad \dot{w}_s = \frac{\dot{w}_s^* L^*}{\rho_{\infty}^* V_{\infty}^2} \]

\[ u, v, w = \frac{u^*, v^*, w^*}{V_{\infty}^*} \quad h = \frac{h^*}{V_{\infty}^2} \quad \mu = \frac{\mu^*}{\mu_{\infty}^*} \]

\[ \rho = \frac{\rho^*}{\rho_{\infty}^*} \quad M = \frac{M^*}{M_{\infty}^*} \quad \kappa = \frac{\kappa^*}{\kappa_{\infty}^*} \]

\[ T = \frac{T^*}{T_{\infty}^*} \quad C_{p^*} = \frac{C_{p^*}^* T_{\infty}^*}{V_{\infty}^2} \quad D = \frac{D^*}{D_{\infty}^*} \]

(7)

and the other nondimensional quantities appearing in the equations are

\[ Re = \frac{\rho_{\infty}^* V_{\infty}^* L^*}{\mu_{\infty}^*} \quad \beta_2 = \frac{\kappa_{\infty}^* T_{\infty}^*}{\mu_{\infty}^* V_{\infty}^2} \]

\[ \beta_1 = \frac{\kappa_{\infty}^* T_{\infty}^*}{\rho_{\infty}^* V_{\infty}^2} \quad \beta_3 = \frac{\rho_{\infty}^* D_{\infty}^*}{\mu_{\infty}^*} \]

In order to close the system of governing equations, the thermodynamic and transport properties of the constituent gases and the mixture are required. This is discussed next.
Thermodynamic and Transport Properties

The chemical model used in the present calculations is air consisting of molecular oxygen ($O_2$), atomic oxygen ($O$), molecular nitrogen ($N_2$), atomic nitrogen ($N$), nitric oxide ($NO$), ionic nitric oxide ($NO^+$), and electrons ($e^-$). The electrons are eliminated from the species set using the principle of conservation of charge.

**Enthalpy and specific heat**

The enthalpies and specific heats of species $s$ are obtained from the following relations:

$$h^*_s = T^* \cdot C_{1,s}(T^*) + h^0_s; \quad (J/kg)$$

$$C^*_{p,s} = C_{2,s}(T^*); \quad (J/kg \cdot K)$$

Tables of $C_{1,s}$ and $C_{2,s}$ as functions of $T^*$ ($K$) are obtained from Ref. 22. Cubic spline interpolation is used in these tables. The enthalpy and frozen specific heat of the mixture are given by the following expressions:

$$h^*_f = \sum_{s=1}^{n} c_s h^*_s, \quad C^*_{p,f} = \left. \frac{dh^*}{dT} \right|_{c_1, \ldots, c_n} = \sum_{s=1}^{n} c_s \frac{dh^*_s}{dT} = \sum_{s=1}^{n} c_s C^*_{p,s}$$  \hspace{1cm} (8)

where the subscripts on the differentiation indicate that the composition of the mixture is frozen locally.

**Viscosity and thermal conductivity**

The viscosity of species $s$ is calculated from curve fits developed in Ref. 22. These curve fits are of the form:

$$\mu^*_s = 0.1 \exp \left[ (A_s \log_e T^* + B_s) \log_e T^* + C_s \right]; \quad (N \cdot s/m^2)$$
where $A_s$, $B_s$, and $C_s$ are constants. The thermal conductivity of species $s$ is computed using Eucken’s semiempirical formula

$$
\kappa_s^* = \frac{\mu_s^* R^*}{M_s^*} \left( C_{p,s}^* \frac{M_s^*}{R^*} + \frac{5}{4} \right); \quad (W/m\cdot K)
$$

The viscosity and thermal conductivity of the mixture are calculated using Wilke’s semiempirical mixing rule [33]

$$
\mu^* = \sum_{s=1}^{n} X_s \mu_s^*, \quad \kappa^* = \sum_{s=1}^{n} X_s \kappa_s^*
$$

where

$$
X_s = \frac{c_s M_s^*}{M_s^*}, \quad \phi_s = \sum_{r=1}^{n} X_r \left[ 1 + \sqrt{\frac{\mu_s^*}{\mu_r^*}} \left( \frac{M_r^*}{M_s^*} \right)^{1/4} \right] \left[ \sqrt{8} \sqrt{1 + \frac{M_s^*}{M_r^*}} \right]^{-1}
$$

Wilke’s mixing rule is considered adequate for weakly ionizing flows.

**Diffusion coefficient**

The binary Lewis numbers for all the species are assumed to be the same constant $\mathcal{L}e$. The kinematic binary diffusion coefficient $D^*$ is then computed from the definition

$$
D^* = \frac{\kappa^* \mathcal{L}e}{\rho C_{p,f}^*}; \quad (m^2/s)
$$

The dimensional thermodynamic and transport properties are nondimensionalized using Eq. 7 prior to their use in the computations.

**Coordinate Transformation**

The discretization of Eq. 1 over an arbitrarily shaped solution domain is difficult. Therefore, the physical domain is mapped to an equispaced rectangular
computational domain through the following transformation of spatial coordinates

\[ \xi = \xi(x,y,z), \quad \eta = \eta(x,y,z), \quad \zeta = \zeta(x,y,z) \]

where \( \xi \) is the "streamwise" coordinate, \( \eta \) is the "normal" coordinate and \( \zeta \) is the "circumferential" coordinate. Applying this transformation to Eq. 1, the governing equations can be recast into the strong conservation-law form given by

\[ \frac{\partial}{\partial t} \left( \overline{E}_\xi^i + \overline{F}_\eta^i + \overline{G}_\zeta^i \right) = \frac{1}{Re} \left( \overline{E}_\xi^v + \overline{F}_\eta^v + \overline{G}_\zeta^v \right) + \overline{W}^c \quad (11) \]

where \( \overline{E}_\xi^i, \overline{F}_\eta^i, \overline{G}_\zeta^i, \overline{E}_\xi^v, \overline{F}_\eta^v, \overline{G}_\zeta^v \), and \( \overline{W}^c \), are the transformed inviscid and viscous fluxes and chemical source terms, respectively. These fluxes and source terms are given by

\[ \overline{E}_\xi^i = (\xi_x)E^i + (\xi_y)F^i + (\xi_z)G^i \quad \overline{E}_\xi^v = (\xi_x)E^v + (\xi_y)F^v + (\xi_z)G^v \]
\[ \overline{F}_\eta^i = (\eta_x)E^i + (\eta_y)F^i + (\eta_z)G^i \quad \overline{F}_\eta^v = (\eta_x)E^v + (\eta_y)F^v + (\eta_z)G^v \]
\[ \overline{G}_\zeta^i = (\zeta_x)E^i + (\zeta_y)F^i + (\zeta_z)G^i \quad \overline{G}_\zeta^v = (\zeta_x)E^v + (\zeta_y)F^v + (\zeta_z)G^v \]
\[ \overline{W}^c = \frac{1}{J} \overline{W}^c \quad J = \frac{\partial (\xi, \eta, \zeta)}{\partial (x, y, z)} \]

where \( J \) is the Jacobian of the coordinate transformation. The metrics are given by the expressions

\[ \frac{\xi_x}{J} = (y_\zeta z_\eta - y_\eta z_\zeta) \quad \frac{\xi_y}{J} = (x_\zeta z_\eta - x_\eta z_\zeta) \quad \frac{\xi_z}{J} = (x_\eta y_\zeta - x_\zeta y_\eta) \]
\[ \frac{\eta_x}{J} = (y_\zeta z_\eta - y_\eta z_\zeta) \quad \frac{\eta_y}{J} = (x_\zeta z_\eta - x_\eta z_\zeta) \quad \frac{\eta_z}{J} = (x_\eta y_\zeta - x_\zeta y_\eta) \]
\[ \frac{\zeta_x}{J} = (y_\zeta z_\eta - y_\eta z_\zeta) \quad \frac{\zeta_y}{J} = (x_\zeta z_\eta - x_\eta z_\zeta) \quad \frac{\zeta_z}{J} = (x_\eta y_\zeta - x_\zeta y_\eta) \]
and the Jacobian, \( J \), is calculated using

\[
J = [x_\xi(y_\eta z_\xi - y_\xi z_\eta) + x_\zeta(y_\xi z_\zeta - y_\zeta z_\xi) + x_\eta(y_\zeta z_\eta - y_\eta z_\zeta)]^{-1}
\]

Parabolized Navier-Stokes (PNS) Equations

The equation set, Eq. 11, is simplified by making the thin-layer approximation, i.e., the viscous and diffusion effects in the streamwise and meridional directions are assumed to be negligibly small compared to those in the normal direction. This assumption is valid for high Reynolds number flows. Therefore, the set of equations is reduced to

\[
\ddot{E}^i_\xi + \ddot{F}^i_\eta + \ddot{G}^i_\zeta = \frac{1}{Re} \ddot{F}^v_\eta + \dddot{W}^v
\]

where \( \dddot{F}^v \) contains derivatives with respect to the \( \eta \) coordinate only. This thin-layer viscous flux is

\[
\dddot{F}^v = J \begin{pmatrix}
0 \\
\ell_1 u_\eta + \ell_4 v_\eta + \ell_5 w_\eta \\
\ell_4 u_\eta + \ell_2 v_\eta + \ell_6 w_\eta \\
\ell_5 u_\eta + \ell_6 v_\eta + \ell_3 w_\eta \\
\frac{1}{2}(\ell_1 - \ell_7)(u^2)_\eta + \frac{1}{2}(\ell_2 - \ell_7)(v^2)_\eta + \frac{1}{2}(\ell_3 - \ell_7)(w^2)_\eta + \\
\ell_4(uv)_\eta + \ell_5(uw)_\eta + \ell_6(vw)_\eta + \\
\ell_7 H_\eta + \ell_9(c_1)_\eta + \ell_{10}(c_2)_\eta + \ldots + \ell_{n+7}(c_{n-1})_\eta \\
\ell_8(c_1)_\eta \\
\ell_8(c_2)_\eta \\
\vdots \\
\ell_8(c_{n-1})_\eta
\end{pmatrix}
\]
where the coefficients $\ell_1, \ell_2, \ldots, \ell_{n+7}$ are

$$
\ell_1 = \mu \left[ \frac{4}{3} \left( \frac{n_x}{J} \right)^2 + \left( \frac{n_y}{J} \right)^2 + \left( \frac{n_z}{J} \right)^2 \right] \\
\ell_2 = \mu \left[ \left( \frac{n_x}{J} \right)^2 + \frac{4}{3} \left( \frac{n_y}{J} \right)^2 + \left( \frac{n_z}{J} \right)^2 \right] \\
\ell_3 = \mu \left[ \left( \frac{n_x}{J} \right)^2 + \left( \frac{n_y}{J} \right)^2 + \frac{4}{3} \left( \frac{n_z}{J} \right)^2 \right] \\
\ell_4 = \mu \left[ \left( \frac{n_x}{J} \right) \left( \frac{n_y}{J} \right) \right] \\
\ell_5 = \frac{\mu}{3} \left( \frac{n_x}{J} \right) \left( \frac{n_z}{J} \right) \\
\ell_6 = \frac{\mu}{3} \left( \frac{n_y}{J} \right) \left( \frac{n_x}{J} \right) \\
\ell_7 = \frac{\beta_2 \kappa}{C_p} \left( \left( \frac{n_x}{J} \right)^2 + \left( \frac{n_y}{J} \right)^2 + \left( \frac{n_z}{J} \right)^2 \right) \\
\ell_8 = \beta_3 \rho D \left( \left( \frac{n_x}{J} \right)^2 + \left( \frac{n_y}{J} \right)^2 + \left( \frac{n_z}{J} \right)^2 \right) \\
\ell_{s+8} = (\ell_s - \ell_7)(h_s - h_{n-1}) \\
\ell_{s+8} = s = 1, 2, \ldots, n - 1
$$

In its present form, Eq. 12 is hyperbolic-elliptic in the streamwise or marching direction, $\xi$. This is due to the fact that the presence of the entire streamwise pressure gradient term permits signals to be propagated upstream through the subsonic region of the boundary layer. Consequently, a space-marching procedure for an ill-posed initial boundary-value problem represented by Eq. 12 will, in many cases, lead to exponentially growing or "departure" solutions. The technique used to overcome this problem was originally proposed by Vigneron et al. [34] for ideal gases and is extended to chemically reacting flows in this study. In this approach, only a fraction $\omega$ ($0 \leq \omega \leq 1$) of the streamwise pressure gradient is retained. Therefore, the streamwise inviscid flux is separated into two parts,

$$
\overline{E}' = \overline{E}'' + \overline{E}'''
$$

where

$$
\overline{E}'' = \{ \rho \hat{U}, \rho u \hat{U} + \omega p \frac{\xi_z}{J}, \rho v \hat{U} + \omega p \frac{\xi_y}{J}, \rho w \hat{U} + \omega p \frac{\xi_x}{J}, \rho H \hat{U}, \rho c_1 \hat{U}, \ldots, \rho c_{n-1} \hat{U} \}^T
$$
\[ \mathbf{E}'' = (1 - \omega)p\left\{0, \frac{\xi_z}{J}, \frac{\xi_y}{J}, 0, 0, 0, \ldots, 0\right\}^T \]

and

\[ \hat{\mathbf{u}} = (\frac{\xi_z}{J})u + (\frac{\xi_y}{J})v + (\frac{\xi_z}{J})w \]

The equations that are obtained by substituting Eq. 14 into Eq. 12 are referred to as the parabolized Navier-Stokes (PNS) equations. These equations are written as a single vector equation given below

\[ \mathbf{E}''_\xi + F^i + G^i = \frac{1}{Re} \mathbf{E}''_\eta + \mathbf{W}^c - \mathbf{E}''_\xi \tag{15} \]

An eigenvalue analysis (see Appendix B for details) of Eq. 15 shows that the PNS equations are hyperbolic-parabolic in the \( \xi \) direction if and only if (i) there is no axial flow separation in the solution domain, (ii) the local frozen Mach number is greater than unity in the inviscid part of the flow field, and (iii) \( \omega \) is specified according to the relation

\[ \omega = \min \left\{ 1, \sigma M_f^2 \left[ 1 + \chi (M_f^2 - 1) \right]^{-1} \right\} \tag{16} \]

where \( \sigma \) (0.8 \( \leq \sigma \leq 0.9 \)) is a factor of safety and

\[ \chi = \frac{\beta_1}{MC_{pf}}, \quad M_f = \hat{U} \left[ a_f \left| \frac{\nabla \xi}{J} \right| \right]^{-1}, \quad a_f^2 = \frac{\chi}{(1 - \chi)} C_{pf} T \]

From Eq. 16 it must be noted that the entire pressure gradient term is retained if the local frozen Mach number is greater than unity. The last term of Eq. 15 represents that part of the pressure gradient which introduces ellipticity into the
system and is normally neglected. Hence, the final set of equations that is solved numerically is

\[
\tilde{E}'_s + \tilde{F}_\eta^i + \tilde{G}_s^i = \frac{1}{Re} \tilde{F}_\eta^v + \tilde{W}^c
\]  

(17)
CHAPTER 3. TWO-DIMENSIONAL FLOWS

Two-Dimensional/Axisymmetric PNS Equations

In this part of the study, the steady laminar reacting flow of an n-component gas mixture over two-dimensional/axisymmetric bodies is considered. The PNS equations for this flow are obtained from Eq. 17 and are

\[ \mathbf{E}^{i\prime} + \mathbf{F}^{i} + \mathbf{S}^{i} = \frac{1}{Re} \left( \mathbf{F}^{v} \right)_{n} + \frac{1}{Re} \mathbf{S}^{\nu} + \mathbf{W}^{c} \]  \hspace{1cm} (18)

where the generalized "streamwise" coordinate \( \xi \) and the "normal" coordinate \( \eta \) are related to the Cartesian coordinates \((x, z)\) through the transformation

\[ \xi = \xi(x, z), \quad \eta = \eta(x, z) \]

The \((n + 3)\)-component vector of conservation variables \( Q \) is

\[ Q = \{ \rho, \rho u, \rho w, \rho H, \rho c_{1}, \rho c_{2}, \ldots, \rho c_{n-1} \}^{T} \]  \hspace{1cm} (19)

The \((n + 3)\)-component inviscid flux vectors \( \mathbf{E}^{i} \) and \( \mathbf{F}^{i} \) are

\[ \mathbf{E}^{i} = \{ \rho \dot{U}, \rho u \dot{U} + \omega \rho \frac{\xi_{x}}{J}, \rho w \dot{U} + \omega \rho \frac{\xi_{z}}{J}, \rho H \dot{U}, \rho c_{1} \dot{U}, \ldots, \rho c_{n-1} \dot{U} \}^{T} \]

\[ \mathbf{F}^{i} = \{ \rho \dot{W}, \rho u \dot{W} + \rho \frac{\eta_{x}}{J}, \rho w \dot{W} + \rho \frac{\eta_{z}}{J}, \rho H \dot{W}, \rho c_{1} \dot{W}, \ldots, \rho c_{n-1} \dot{W} \}^{T} \]

where the contravariant velocity components are

\[ \dot{U} = \left( \frac{\xi_{x}}{J} \right)u + \left( \frac{\xi_{z}}{J} \right)w, \quad \dot{W} = \left( \frac{\eta_{x}}{J} \right)u + \left( \frac{\eta_{z}}{J} \right)w \]
The \((n + 3)\)-component thin-layer viscous flux vector \(\mathbf{F}^v\) is

\[
\mathbf{F}^v = \frac{1}{J} \begin{pmatrix}
0 \\
\ell_1 u_n + \ell_2 w_n \\
\ell_3 u_n + \ell_2 w_n \\
\frac{1}{2}(\ell_1 - \ell_4)(u^2)_n + \frac{1}{2}(\ell_2 - \ell_4)(w^2)_n + \ell_3(\mu w)_n + \\
\ell_4 H_n + (\ell_5 - \ell_4) \sum h_s(c_s)_n \\
\ell_5(c_1)_n \\
\ell_5(c_2)_n \\
\vdots \\
\ell_5(c_{n-1})_n
\end{pmatrix}
\]

where the coefficients \(\ell_1\) through \(\ell_5\) are

\[
\ell_1 = \mu \left( \frac{4}{3} \eta_x^2 + \eta_z^2 \right) \\
\ell_2 = \mu \left( \eta_x^2 + \frac{4}{3} \eta_z^2 \right) \\
\ell_3 = \mu \left( \frac{1}{3} \eta_x \eta_z \right)
\]

The inviscid source vector, \(\mathbf{S}^i\), for the axisymmetric formulation is

\[
\mathbf{S}^i = \frac{1}{zJ} \{ \rho w, \rho u w, \rho w^2, \rho w H, \rho w c_1, \rho w c_2, \ldots, \rho w c_{n-1} \}^T
\]

the viscous source vector, \(\mathbf{S}^v\), for the axisymmetric formulation is

\[
\mathbf{S}^v = \frac{1}{zJ} \begin{pmatrix}
0 \\
-\frac{2}{3} \eta_z(\mu w/z)_n + \mu(\eta z w_n + \eta z u_n) \\
-\frac{2}{3} \eta_x(\mu u w/z)_n + 2\mu(\eta x w_n - w/z) \\
-\frac{2}{3} \eta z(\mu u w/z)_n - \frac{2}{3} \eta z(\mu w^2)_n + \\
\frac{1}{2}(\mu + \frac{\partial \kappa}{C_p}) \eta_x(u^2 + w^2)_n + \mu(\eta x u_n + \eta x w_n) - \\
\frac{3}{2} \mu w(\eta z u_n + \eta z w_n)_n - \frac{\beta \kappa}{C_p} \eta z H_n + \\
(\frac{\partial \kappa}{C_p} - \beta_3 \rho D) \eta z \sum h_s(c_s)_n \\
\beta_3 \rho D \eta z(c_1)_n \\
\beta_3 \rho D \eta z(c_2)_n \\
\vdots \\
\beta_3 \rho D \eta z(c_{n-1})_n
\end{pmatrix}
\]
and the chemical source vector, $\overline{W}^x$, is

$$\overline{W}^x = \frac{1}{J} \{0, 0, 0, 0, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_{n-1}\}^T$$

The expressions for the Jacobian, $J$, and the metrics of the coordinate transformation, $\xi_z$, $\xi_x$, $\eta_z$, and $\eta_x$ are

$$J = \frac{\partial(\xi, \eta)}{\partial(x, z)} = \left( x_{\xi z \eta} - x_{\eta z \xi} \right)^{-1}$$

$$\frac{\xi_z}{J} = z_n \quad \frac{\eta_z}{J} = -x_z$$

$$\frac{\xi_x}{J} = -x_\eta \quad \frac{\eta_x}{J} = x_\xi$$

Gas Model and Reactions

The chemical model used in the present calculations is air consisting of molecular oxygen ($O_2$), atomic oxygen ($O$), atomic nitrogen ($N$), nitric oxide ($NO$), and molecular nitrogen ($N_2$). These species are indexed $s = 1 - 5$ in the order shown.

The following reactions are considered between the constituent species

1. $O_2 + M_1 \rightleftharpoons 2O + M_1$
2. $N_2 + M_2 \rightleftharpoons 2N + M_2$
3. $N_2 + N \rightleftharpoons 2N + N$
4. $NO + M_3 \rightleftharpoons N + O + M_3$
5. $NO + O \rightleftharpoons O_2 + N$
6. $N_2 + O \rightleftharpoons NO + N$

where $M_1$, $M_2$, and $M_3$ are catalytic third bodies. The above model has five species ($n = 5$), six reactions ($m = 6$) and eight reactants ($n_t = 8$). The mass production
rate of any species \( s \) of the gas model is calculated using expressions developed in Appendix A and all the necessary rate constants are obtained from Ref. 22.

**Finite-Difference Algorithm**

An implicit, noniterative finite-difference scheme is used to solve the system of equations, Eq. 18. This algorithm is an adaptation of the one developed by Tannehill et al. [35]. The algorithm in delta-form is

\[
\left\{ \hat{A}_{i,k} + \Delta \xi \frac{\partial}{\partial \eta} \left( \hat{B}_{i,k} - \frac{1}{Re} \hat{M}_{i,k} \right) - D_1 \right\} \Delta Q_{i,k} = -\Delta \xi \bar{E}_{\xi}^{i'} |_Q \\
-\Delta \xi \left\{ \frac{\partial}{\partial \eta} \left( \bar{F}_{i,k}^{i'} - \frac{1}{Re} \bar{F}_{i,k}^{v'} \right) + \bar{S}_{i,k}^{i'} - \frac{1}{Re} \bar{S}_{i,k}^{v'} - [\bar{W}_{i,k}^{c'}] \right\} + D_2 \bar{E}_{\xi}^{v'} \\
Q_{i+1,k} = Q_{i,k} + \Delta Q_{i,k}
\]

where

\[
\hat{A} = \left( \frac{\partial \bar{E}_{\xi}^{i'}}{\partial Q} \right), \quad \hat{B} = \left( \frac{\partial \bar{F}_{i,k}^{i'}}{\partial Q} \right), \quad \hat{M} = \left( \frac{\partial \bar{F}_{i,k}^{v'}}{\partial Q} \right)
\]

The subscript \( i \) refers to the station \( \xi = i \Delta \xi \) and the subscript \( k \) refers to the point \( \eta = (k-1) \Delta \eta \). The derivative \( \partial / \partial \eta \) is replaced by the conventional three-point central-difference operator. The algorithm is first-order accurate in the \( \xi \) direction and second-order accurate in the \( \eta \) direction.

The Jacobian matrices \( \hat{A}, \hat{B} \) and \( \hat{M} \) can be derived as shown in Appendices C and D. In the linearization of the viscous flux, the transport properties are assumed to be locally constant. All the source terms have been lagged in the present formulation.
The left hand side of Eq. 20 corresponds to a block-tridiagonal system of equations. The blocks are square matrices of order \((n + 3)\). For the five-species air model considered in the present calculations, the blocks are square matrices of order 8. The block-tridiagonal solver for the \(8 \times 8\) blocks is developed along the same lines as the one by Steger [36] for \(5 \times 5\) blocks.

\(D_1\) and \(D_2\) are second-order implicit and fourth-order explicit smoothing operators, respectively. These operators have the following forms

\[
D_1 = \varepsilon_1 \frac{1}{J_{i,k}} \left[ \Delta_n \nabla_n (J_{i,k} \hat{A}_{i,k}) \right] 
\]

\[
D_2 = \varepsilon_2 \frac{|p_{i,k+1} - 2p_{i,k} + p_{i,k-1}|}{(p_{i,k+1} + 2p_{i,k} + p_{i,k-1})} \left( \Delta_n \nabla_n \right) 
\]

where \(\varepsilon_1, \varepsilon_2\) are constants to be specified by the user. \(\Delta_n\) and \(\nabla_n\) are the conventional forward and backward difference operators, respectively.

Boundary and Initial Conditions

In the present work, the outer boundary is taken to be the freestream and the wall is taken to be the inner boundary. Any discontinuities in the flowfield are “captured” as a part of the solution.

The following nondimensional boundary conditions are imposed implicitly at the wall:

(a) \(u = 0, \ v = 0, \ \frac{\partial}{\partial n} (p) = 0\)

(b) \(T = T_w\) (isothermal wall) or \(\frac{\partial}{\partial n} (T) = 0\) (adiabatic wall)

(c) \(c_s = c_{s\infty}\) (catalytic wall) or \(\frac{\partial}{\partial n} (c_s) = 0\) (noncatalytic wall), \(s = 1, 2, \ldots, n - 1\)
The nondimensional boundary conditions at the outer boundary are

(a) \( u = 1, \ v = 0 \)

(b) \( T = 1, \ \rho = 1, \ c_s = c_{s_{\infty}}, \ s = 1,2, \ldots, n - 1 \)

The PNS equations require initial conditions in addition to the boundary conditions. The usual procedure is to use an initial data plane generated by a full Navier-Stokes code. For conical or pointed bodies, however, the code generates its own starting solution. This starting solution is generated iteratively using a “stepback” procedure [37]. In this procedure, the viscous flow is assumed to be conical. Such an assumption is approximately valid for high Reynolds number flows over pointed bodies. The flow variables are set to their freestream values and the solution plane is marched from \( \xi = \xi_0 \) to \( \xi = \xi_0 + \Delta \xi \) on a conical grid. The variables at the new station are scaled back to \( \xi = \xi_0 \). This procedure is continued until the \( L_2 \)-norm of the change in variables is less than a preset tolerance.

Decoding

The primitive variables, \( \rho, u, w, H, c_1, \ldots, c_{n-1} \), at station \( i + 1 \) are easily obtained from the elements of \( Q_{i+1,k} \). The mass fraction of the \( n \)th species is computed using Eq. 3 and the static enthalpy of the mixture is computed using Eq. 5. For a given species distribution \( c_1, c_2, \ldots, c_n \) and mixture enthalpy \( h \) the following is true

\[
    h^* = \sum_{s=1}^{n} c_s h_s^*(T^*) = g(T^*)
\]

The only unknown in the above equation is the temperature. To determine this
temperature the Newton-Raphson (NR) method is employed because the method converges quadratically. The NR algorithm is

\[ T^{*k+1} = T^{*k} - \frac{\frac{g(T^{*k})}{g'(T^{*k})} - h^*}{g'(T^{*k})} \]

where \( k \) is the index of iteration and ' indicates differentiation with respect to the variable \( T^* \). The function \( g'(T^*) \) is simply the frozen specific heat of the mixture. Therefore, the iteration scheme becomes

\[ T^{*k+1} = T^{*k} - \frac{\sum_{s=1}^{n} c_s h_s^*(T^{*k}) - h^*}{\sum_{s=1}^{n} c_s C_p^s(T^{*k})} \]  

(23)

The iterations are continued until the absolute value of the difference between two successive values of temperature is less than a given tolerance. Once the temperature is determined, the thermodynamic and transport properties are easily computed using the expressions given in the previous sections.

Grid Generation

An algebraic grid generation procedure is used in the present calculations. In this procedure, the point on the body surface and the point on the outer boundary are connected by a straight line and the grid points are distributed on this line using the following stretching function

\[ s(\eta) = 1 - \beta \left\{ \frac{(\beta + 1)^{1-n} - (\beta - 1)^{1-n}}{(\beta + 1)^{1-n} + (\beta - 1)^{1-n}} \right\} \]  

(24)

\[ \eta = \frac{(k - 1)}{(NK - 1)} \quad k = 1, 2, \ldots, NK \]  

(25)
where $\beta (\beta > 1)$ is the stretching parameter and $NK$ the total number of points on the grid line. Note that $s(0) = 0$ and $s(1) = 1$ and the points are clustered close to the wall for values of $\beta$ close to 1. Such clustering is necessary for good resolution of the subsonic viscous layer.

The coordinates of the grid points are obtained from

$$x(\xi, \eta) = x_\omega(\xi) + s(\eta)n_1(\xi)\delta(\xi)$$

$$y(\xi, \eta) = y_\omega(\xi) + s(\eta)n_2(\xi)\delta(\xi)$$

(26)

where $n_1$ and $n_2$ are the direction cosines of the unit vector along the grid line and $\delta$ is the linear distance of the outer boundary from the body surface.

The metrics are then computed using one-sided differences in the $\xi$ direction and central-differences in the $\eta$ direction.

**Results**

In order to validate the present PNS code for chemical nonequilibrium flows, two test cases were computed. The coordinate system employed in the present calculations is shown in Fig. 1.

**Test Case 1. Wedge**

The first test case computed was that of hypersonic laminar flow of dissociating air over a 10 degree wedge. The altitude chosen was 60.96 km where the ambient pressure and temperature are 20.35 $N/m^2$ and 252.6 $K$, respectively. The remaining flow conditions were

$$V_\infty^* = 8100 \ m/s$$

$$T_w^* = 1200 \ K$$

and noncatalytic wall
Figure 1. Coordinate system
ci = 0.21 and C5 = 0.79
Le = 1.4

The computation was started at \(x^*/L^* = 10^{-3}\). The initial conditions were chosen to be the freestream conditions and the “stepback” procedure was used to obtain a converged initial solution. This initial solution was marched to \(x^*/L^* = 3.5\). The nondimensional marching step size was varied linearly from \(5 \times 10^{-4}\) to \(1.2 \times 10^{-3}\). The grid used in the calculations consisted of 67 points in the normal direction. The nondimensional distance of the first point away from the body surface was also varied linearly from \(8 \times 10^{-5}\) to \(3.5 \times 10^{-4}\) which determined the appropriate stretching parameter \(\beta\). The grid lines were placed normal to the body and the nondimensional height of the outer boundary was kept fixed at 0.75. The edge of the boundary layer was located approximately using total enthalpy as the criterion. The edge values of pressure, temperature and velocity at the last station were then used as the uniform edge conditions for the reacting boundary-layer (RBL) code of Ref. 22.

Profiles of tangential velocity and temperature at \(x^*/L^* = 3.5\) obtained from the two codes are compared in Figs. 2 and 3, respectively. The tangential velocity is defined as

\[
U_t = U \cdot \cos \theta + \dot{w} \cdot \sin \theta
\]  

(27)

The agreement between the two codes is very good except over a small distance close to the boundary-layer edge. The \(O\) mass fraction and \(NO\) mass fraction at
Figure 2. Tangential velocity profiles at $x^*/L^* = 3.5$
Figure 3. Temperature profiles at $x^* / L^* = 3.5$
The nondimensional pressure, skin-friction, and heat transfer coefficients are defined as follows

\[ C_p = \frac{p_w}{\frac{1}{2} \rho_{ref} V_{ref}^2} \quad C_f = \frac{\tau_w}{\frac{1}{2} \rho_{ref} V_{ref}^2} \quad C_h = \frac{-q_w}{\frac{1}{2} \rho_{ref} V_{ref}^3} \]  \hspace{1cm} (28)

where the wall shear stress is computed from

\[ \tau_w = -\mu_w \frac{\partial V^*}{\partial n^*} \bigg|_w \]  \hspace{1cm} (N/m²)  \hspace{1cm} (29)

and the total heat transfer is computed from

\[ q_w = -\kappa_w \frac{\partial T^*}{\partial n^*} \bigg|_w - \rho_w c_w \sum_{s=1}^{n} \frac{\partial c_s}{\partial n^*} \bigg|_w \]  \hspace{1cm} (W/m²)  \hspace{1cm} (30)

The first term in Eq. 30 is the conductive heating rate and the second term is the diffusive heating rate. The partial derivative, \( \partial \)/\( \partial n^* \), is taken in the direction normal to the surface of the body.
Figure 4. $O$ mass fraction profiles at $x^*/L^* = 3.5$
Figure 5. NO mass fraction profiles at $x^* / L^* = 3.5$
For this test case the freestream conditions were chosen to be the reference conditions. In Fig. 6, the wall pressure coefficient is plotted against the axial distance. It is evident from this figure that the pressure predicted by the PNS code is higher than the edge pressure of the RBL code. It is also clearly seen that this pressure asymptotically reaches the edge pressure of the RBL code. The heat transfer and skin-friction coefficients obtained from the two codes are plotted as functions of the distance along the code axis in Figs. 7 and 8, respectively. The coefficients predicted by the two codes are in excellent agreement.

Test Case 2. Cone

The second test case computed was that of hypersonic laminar flow of dissociating air over a 10 degree cone at two different altitudes. The first altitude chosen was 60.96 km where the ambient pressure and temperature are 20.35 N/m² and 252.6 K, respectively and the second altitude chosen was 45.72 km where the ambient pressure and temperature are 136.7 N/m² and 266.2 K, respectively. The remaining flow conditions were

\[ V_\infty = 8100 \text{ m/s} \]

\[ T_w^* = 1200 \text{ K} \text{ and noncatalytic wall} \]

\[ c_{1\infty} = 0.21 \text{ and } c_{3\infty} = 0.79 \]

\[ Le = 1.4 \]

The computations for both the altitudes were started at \( x^*/L^* = 10^{-2} \). The initial conditions were chosen to be the freestream conditions and the "stepback"
Figure 6. Wall pressure coefficient comparison
Figure 7. Heat transfer coefficient comparison
Figure 8. Skin-friction coefficient comparison
procedure was used to obtain converged initial solutions. These initial solutions were marched to $x^*/L^* = 3.5$. The grids used in both the calculations consisted of 67 points in the normal direction. For the higher altitude, the nondimensional marching step size was varied linearly from $5 \times 10^{-4}$ to $1.2 \times 10^{-3}$, the nondimensional distance of the first point away from the body surface was varied linearly from $8 \times 10^{-5}$ to $3.5 \times 10^{-4}$, the grid lines were placed normal to the body, and the nondimensional height of the outer boundary was kept fixed at 0.5. For the lower altitude, the marching step size was varied linearly from $1 \times 10^{-5}$ to $1.2 \times 10^{-3}$, the distance of the first point away from the body surface was varied linearly from $5 \times 10^{-6}$ to $7 \times 10^{-5}$, the grid lines were placed normal to the body and the height of the outer boundary was kept fixed at 0.35. As in the previous test case, the edge of the boundary layer was located approximately using total enthalpy as the criterion and the edge values of pressure, temperature and velocity at the last station were then used as the uniform edge conditions for the RBL code of Ref. 22.

The tangential velocity and temperature profiles at $x^*/L^* = 3.5$ obtained from the two codes are plotted in Figs. 9 and 10, respectively. The agreement between the two codes is excellent for both the altitudes. The velocity and thermal boundary layers corresponding to the lower altitude are much thinner than those at the higher altitude. This is to be expected because the lower altitude corresponds to a higher Reynolds number. The $O$ mass fraction and $NO$ mass fraction profiles at $x^*/L^* = 3.5$ obtained from the two codes are displayed in Figs. 11 and 12,
Figure 9. Tangential velocity profiles at $x^* / L^* = 3.5$.
Figure 10. Temperature profiles at $x^*/L^* = 3.5$
Figure 11. $O$ mass fraction profiles at $x''/L'' = 3.5$
Figure 12. NO mass fraction profiles at $x^*/L^* = 3.5$
respectively. The amount of NO predicted by the PNS code is higher than that predicted by the boundary-layer code for the higher altitude. For the lower altitude the amounts of NO predicted by the two codes are in good agreement. As mentioned earlier, the lower altitude corresponds to a higher Reynolds number and consequently, the viscous boundary layer is quite thin. The interaction between the inviscid outer flow and the inner boundary layer is not as strong as that at the higher altitude.

The freestream conditions corresponding to the lower altitude were chosen as the reference conditions for the nondimensional coefficients. The computed surface pressure coefficients at the two altitudes are plotted as functions of the distance along the cone axis in Fig. 13. It is clearly seen from the figure that the surface pressure asymptotically reaches a constant value. In Figs. 14 and 15, the computed heat transfer and skin-friction coefficients, respectively, are displayed as functions of the axial distance. The agreement between the two codes is excellent at both altitudes. It is also evident from the figures that the heat transfer and skin-friction at the lower altitude are larger than those at the higher altitude.

In Fig. 16, the peak temperature in the viscous boundary layer is plotted as a function of the axial distance. The peak temperatures at the lower altitude are smaller than those at the higher altitude. This is to be expected since more dissociation takes place at the lower altitude. The peak O, N, and NO mass fractions in the flow field are plotted against the axial distance in Figs. 17-19,
Figure 13. Wall pressure coefficient comparison
Figure 14. Heat transfer coefficient comparison
Figure 15. Skin-friction coefficient comparison
Figure 16. Axial variation of peak temperature
Figure 17. Axial variation of peak O mass fraction
Figure 18. Axial variation of peak $N$ mass fraction
Figure 19. Axial variation of peak NO mass fraction
respectively. As seen in these figures, significantly more dissociation takes place at the lower altitude than at the higher altitude.

All the computations were performed on the CRAY-XMP/48 computer at NASA Ames Research Center. Each test case involved $8 \times 8$ block matrices and required 0.2 milliseconds per grid point per step. The first test case required 4100 steps and the second test case required 4100 and 5800 steps for the higher and lower altitudes, respectively.
CHAPTER 4. THREE-DIMENSIONAL FLOWS

The feasibility of computing chemical nonequilibrium flow fields using the coupled approach was established in the previous chapter by successfully computing two-dimensional/axisymmetric flows of reacting air. Having done so, a three-dimensional PNS code for chemically reacting flow fields was then developed. The equations governing the flow, repeated here for the sake of completeness, are

\[ \Phi_t^i + \Phi_\eta^i + \Omega_s^i = \frac{1}{Re} \Phi_\eta^\nu + \Phi^c \]  \hspace{1cm} (31)

Gas Model and Reactions

The chemical model used in the present calculations is air consisting of molecular oxygen \((O_2)\), atomic oxygen \((O)\), atomic nitrogen \((N)\), nitric oxide \((NO)\), nitric oxide ion \((NO^+)\), molecular nitrogen \((N_2)\), and electrons \((e^-)\). These species are indexed \(s = 1 - 6\) in the order shown. The electrons are eliminated from the main species set using the principle of conservation of charge. The following reactions are considered between the constituent species

1. \[ O_2 + M_1 \rightleftharpoons 2O + M_1 \]
2. \[ N_2 + M_2 \rightleftharpoons 2N + M_2 \]
3. \[ N_2 + N \rightleftharpoons 2N + N \]
4. \[ NO + M_3 \rightleftharpoons N + O + M_3 \]
5. \[ NO + O \rightleftharpoons O_2 + N \]
6. \[ N_2 + O \rightleftharpoons NO + N \]
7. \[ N + O \rightleftharpoons NO^+ + e^- \]

where \(M_1, M_2,\) and \(M_3\) are catalytic third bodies. The above model has six species \((n = 6)\), seven reactions \((m = 7)\) and ten reactants \((n_t = 10)\) including electrons. The necessary reaction rate constants are obtained from Blottner et al. [22].
Finite-Difference Algorithm

The numerical algorithm used to solve the system of equations, Eq. 31, is once again an adaptation of the one developed by Tannehill et al. [35]. The factored algorithm is implemented as the following sequence of steps

\[
\begin{align*}
\{ \overline{A}_{i,k,j} + \Delta \xi \frac{\partial}{\partial \xi} (\hat{C}_{i,k,j}) \} \Delta \overline{Q}_{i,k,j} &= -\Delta \xi \overline{E}_i^\xi \\
\Delta \xi \left[ \frac{\partial}{\partial \eta} \left( \hat{F}^i_{i,k,j} - \frac{1}{Re} \hat{F}^v_{i,k,j} \right) + \frac{\partial}{\partial \xi} (\hat{G}^i_{i,k,j}) \right] + \Delta \xi \hat{W}^c_{i,k,j} \\
\{ \overline{A}_{i,k,j} + \Delta \xi \frac{\partial}{\partial \eta} (\hat{B}_{i,k,j} - \frac{1}{Re} \hat{M}_{i,k,j}) \} \Delta Q_{i,k,j} &= \overline{A}_{i,k,j} \Delta \overline{Q}_{i,k,j} \quad (32)
\end{align*}
\]

\[
Q_{i+1,k,j} = Q_{i,k,j} + \Delta Q_{i,k,j} \quad (33)
\]

where

\[
\overline{A} = \hat{A} - \Delta \xi \hat{A}^c
\]

and where the Jacobian matrices are

\[
\begin{align*}
\hat{A} &= \frac{\partial \hat{E}_i^v}{\partial Q}, \quad \hat{B} = \frac{\partial \hat{F}_i^v}{\partial Q}, \quad \hat{C} = \frac{\partial \hat{G}_i^v}{\partial Q} \\
\hat{M} &= \frac{\partial \hat{F}_i^v}{\partial Q}, \quad \hat{A}^c = \frac{\partial \hat{W}^c}{\partial Q}
\end{align*}
\]

The subscripts \(i, k, j\) are indices associated with the directions \(\xi, \eta, \zeta\), respectively. \(\Delta \xi\) is the marching stepsize. The derivatives \(\partial/\partial \eta\) and \(\partial/\partial \zeta\) are replaced by conventional three-point central-difference operators. The algorithm is first-order accurate in the \(\xi\) direction and second-order accurate in the \(\eta\) and \(\zeta\) directions. Freestream fluxes are subtracted from the inviscid fluxes in order to preserve freestream. Fourth-difference explicit and second-difference implicit smoothing operators are also added to the factored operators. Their forms are given by Eqs. 21 and 22.
The Jacobian matrices $\hat{A}$, $\hat{B}$, $\hat{C}$, $\hat{M}$, and $\hat{A}^c$ represent the linearization of the fluxes and source terms and the elements of these matrices are derived in Appendices C, D, and E. In the linearization of the viscous flux, the transport properties are assumed to be locally constant. The caret above the symbols for the fluxes, Jacobians, and source terms signifies that the geometry is not linearized along with the flow variables.

The left hand sides of Eqs. 32 and 33 correspond to a block-tridiagonal system of equations. The blocks are square matrices of order $(n + 4)$. For the six-species air model considered in the present calculations, the blocks are square matrices of order 10. The block-tridiagonal solver for the $10 \times 10$ blocks is developed along the same lines as the one by Steger [36] for $5 \times 5$ blocks.

Boundary and Initial Conditions

In the present work, only flows without yaw are considered. Therefore, at every streamwise station the computational domain is bounded by (i) the outer boundary which is taken to be the freestream, (ii) the inner boundary which is taken to be the wall, and (iii) the pitch plane of symmetry. Any discontinuities in the flowfield are “captured” as a part of the solution.

At the pitch plane of symmetry reflection boundary conditions are imposed and thus, flow symmetry is maintained.

The following nondimensional boundary conditions are imposed implicitly at the wall

(a) $u = 0, \ v = 0, \ w = 0, \ \frac{\partial}{\partial n} (p) = 0$
(b) $T = T_w$ (isothermal wall) or $\frac{\partial}{\partial n} (T) = 0$ (adiabatic wall)
(c) $c_s = c_{s\infty}$ (catalytic wall) or $\frac{\partial}{\partial n} (c_s) = 0$ (noncatalytic wall), $s = 1, 2, \ldots, n - 1$

The nondimensional boundary conditions at the outer boundary are
(a) $u = \cos \alpha, \ v = 0, \ w = \sin \alpha$

(b) $T = 1, \ \rho = 1, \ c_s = c_{s\infty}, \ s = 1, 2, \ldots, n - 1$

The initial conditions for the PNS equations are usually obtained using a time-dependent Navier-Stokes solver. The code generates its own starting solution for conical or pointed bodies using an iterative scheme previously referred to as a "stepback" procedure [37].

In order to evaluate the thermodynamic and transport properties of the mixture, the static temperature is necessary. Knowing the species distributions and mixture static temperature, this temperature is determined iteratively using the Newton-Raphson algorithm given by Eq. 23.

Grid Generation

In this part of the study too, an algebraic grid generation procedure is used. Recall that in this procedure, the point on the body surface and the point on the outer boundary are connected by a straight line and the grid points are distributed on this line using the stretching function given by Eq. 24.

The coordinates of the grid points are then obtained from

$$
\begin{align*}
    x &= x_w + n_1 s(\eta) \delta(\xi) \\
    y &= y_w + n_2 s(\eta) \delta(\xi) \\
    z &= z_w + n_3 s(\eta) \delta(\xi)
\end{align*}
$$

where $n_1, n_2,$ and $n_3$ are the direction cosines of the unit vector along the grid line and $\delta$ is the linear distance of the outer boundary from the body surface.

The metrics are then computed using first-order accurate one-sided differences in the $\xi$ direction and second-order accurate central-differences in the $\eta$ and $\zeta$ directions.
Results

In order to validate the present three-dimensional nonequilibrium PNS code, two test cases were computed.

Test Case 1. Axisymmetric cone

The first test case computed was that of hypersonic laminar flow of dissociating air over a 10 degree cone at 0 degree angle of attack. The altitude chosen was 60.96 km where the ambient pressure and temperature are 20.35 N/m² and 252.6 K, respectively. The remaining flow conditions are

\[ V_\infty = 8100 \text{ m/s} \]
\[ T_\infty = 1200 \text{ K and noncatalytic wall} \]
\[ c_{1,\infty} = 0.2629 \text{ and } c_{3,\infty} = 0.7371 \]
\[ \mathcal{L}e = 1.4 \]

The computation was started at \( x^*/L^* = 1.5 \times 10^{-3} \) using the initial solution generated by the "stepback" procedure. The solution was then marched to \( x^*/L^* = 3.5 \). The marching step size was chosen to be \( \Delta \xi = f\delta_s \) where \( f > 1 \) and \( \delta_s \) is the maximum thickness of the subsonic layer (in the present calculations, a value of 2 was assigned to \( f \)). The grid used in the calculations consisted of 67 points in the normal direction and 21 points in the meridional direction. The distance of the first point away from the body surface was varied linearly from \( 3 \times 10^{-5} \) to \( 2.3 \times 10^{-4} \) which determined the appropriate stretching parameter \( \beta \). The grid lines were placed normal to the body and the height of the outer boundary was kept fixed at 0.5. The edge of the boundary layer was located approximately using total enthalpy as the criterion. The edge values of pressure, temperature and velocity at the last station were then used as the uniform edge conditions for the reacting boundary-layer (RBL) code of Ref. 22.
The surface pressure coefficient is defined as

\[ C_p = \frac{p_w - p_{\infty}}{\frac{1}{2} \rho_{\infty} V_{\infty}^2} \]  

(35)

In Fig. 20, the axial variation of the surface pressure coefficient is compared against the edge pressure of the boundary-layer code. The pressure predicted by the PNS code is initially higher than the edge pressure of the RBL code but eventually asymptotes to the latter value. The higher pressure is believed due to the leading edge effect. It must be recalled here that the PNS equations contain a normal momentum equation. This permits the interaction of the outer inviscid region with the inner viscous region. At the altitude considered, this interaction is fairly strong because the Reynolds number is low. Consequently, the pressure is higher. As the solution proceeds downstream, the interaction is reduced and one obtains near boundary-layer behavior. The increase in pressure leads to some differences between the PNS and boundary-layer results as will be discussed later.

The PNS equations are uniformly valid in the shock layer and, as mentioned earlier, the solution domain includes both the viscous and inviscid regions. In Figs. 21-26 only 20 percent of the solution domain is shown in order to emphasize the details of the viscous boundary layer. Pitch plane profiles of tangential velocity and temperature at \( x' / L' = 3.5 \) are compared in Figs. 21 and 22, respectively. The agreement between the two codes is excellent. Mass fraction profiles of \( O \) and \( NO \) at \( x' / L' = 3.5 \) are compared in Figs. 23 and 24, respectively. The mass fractions have been normalized using the corresponding wall values. The agreement between the two codes is again excellent. The wall values of the mass fractions were also found to be in very good agreement. The electron density (number of electrons per \( m^3 \)) is obtained from the mass fraction of the \( NO^+ \) ion. This follows from charge
Figure 20. Wall pressure coefficient comparison
Figure 21. Tangential velocity profiles at $x^*/L^* = 3.5$
Figure 22. Temperature profiles at $x^*/L^* = 3.5$
Figure 23. $O$ mass fraction profiles at $x^*/L^* = 3.5$
Figure 24. NO mass fraction profiles at $x^*/L^* = 3.5$
conservation and is defined as

\[ N_e^* = \frac{N_{NO^+}^*}{M_{NO^+}^*} \]  

(36)

In Figs. 25 and 26, profiles of the mass fraction of \( NO^+ \) and electron density obtained from the two codes are compared. Again, the mass fractions and densities have been normalized using the corresponding wall values. The curve corresponding to the PNS calculations passes below the symbols representing the boundary-layer calculations. This is due to the fact that the PNS code predicts a higher amount of \( NO^+ \) near the wall. The onset of chemical reactions occurs earlier in the PNS code than in the RBL code because of the initial high pressures. This effect persists downstream and hence the disparity. The electron densities have been obtained from the mass fractions of \( NO^+ \) and consequently these densities will exhibit an identical behavior.

The skin-friction coefficient and the Stanton number are defined as:

\[ C_f = \frac{\tau_w}{\frac{1}{2} \rho_\infty V_\infty^2} \]  

(37)

\[ St = \frac{-q_w}{\rho_\infty V_\infty (H_\infty - H_w)} \]  

(38)

where the wall shear stress and total heat transfer are calculated using Eqs. 29 and 30, respectively. In Figs. 27 and 28, the skin-friction coefficient and Stanton number are plotted as functions of the distance along the cone axis. The coefficients predicted by the two codes are in very good agreement. The total drag coefficient is defined as

\[ C_d = \frac{D^*}{\frac{1}{2} \rho_\infty V_\infty^2 A} \]  

(39)
Figure 25. \( NO^+ \) mass fraction profiles at \( x^*/L^* = 3.5 \)
Figure 26. Electron density profiles at $x^*/L^* = 3.5$
Figure 27. Skin-friction coefficient comparison
Figure 28. Stanton number comparison
where \( D^* (N) \) is the total drag, \( i.e., \) the sum of the pressure drag and the skin-friction drag. The base pressure drag has been neglected. In the present study, trapezoidal integration was used to compute the total drag. The cross-sectional area at \( x''/L'' = 3.5 \) was chosen as the reference area. The value of the drag coefficient predicted by the PNS code was 0.1037 which is in very good agreement (less than 1 percent) with the value of 0.1043 predicted by the RBL code.

The ideal gas and equilibrium air models represent two physical extremes. In the former case, there are no reactions (infinitely slow reactions) and in the latter case, the reactions proceed at an infinite rate. In the gas model considered in the present calculations, the reactions proceed at finite-rate and hence is between these two extremes. In order to demonstrate this, the PNS code of Ref. 38 was modified and specialized to two-dimensional and axisymmetric bodies. New curve fits [39] for the thermodynamic properties of equilibrium air were used in the code. For the ideal gas calculations the ratio of specific heats was set to 1.4. The code was then used to compute the flow around the 10 deg. cone for the same freestream conditions. In Fig. 29, the temperature profiles at \( x''/L'' = 3.5 \) obtained for the three gas models are compared. It is evident from the figure that the peak temperature for the finite-rate chemistry case lies between the peaks for the ideal gas and equilibrium air models. In the ideal gas case there are no internal degrees of freedom for the energy to be stored. For the finite-rate reaction case, some of the energy goes into exciting the internal degrees of freedom and some into chemical reactions. This effectively lowers the peak temperature. For the equilibrium air model, thermochemical equilibrium is achieved, instantaneously at every point of the flow field and hence a much lower peak temperature. In Fig. 30, the effect of the three gas models on the Stanton number is shown. The Stanton number
Figure 29. Temperature profiles at $x^* / L^*$ = 3.5 for various gas models
Figure 30. Axial variation of Stanton number for various gas models
has been plotted as a function of the axial distance. The equilibrium Stanton number is slightly greater than the finite-rate chemistry model which in turn is greater than the ideal gas Stanton number.

**Test Case 2. Circular cone at angles of attack**

In order to validate the angle of attack capability of the code, a simple test case was chosen. In this test case, hypersonic laminar flow of reacting air over a 10 degree cone at 2.5, 5, 7.5 and 10 degrees angle of attack was computed. The flow conditions for these calculations were the same as the flow conditions for Test Case 3. The starting solution for the PNS code for each angle of attack was obtained using the stepback procedure with the guessed initial solution being the freestream. The mesh spacing on the windside had to be progressively refined for each angle of attack in order to properly resolve the boundary layer. The factor $f$ that multiplies the maximum subsonic layer thickness was decreased from 1.8 (2.5 deg case) to 1.25 (10 deg case) to maintain reasonable marching stepsizes. In each case the grid lines were placed orthogonal to the body. The starting solution was marched up to an axial location of $x'/L' = 2.5$. Since there is a paucity of experimental data in such severe hypersonic regimes, the results of these calculations are simply compared against the results of the zero degree calculations.

The computed results for this test case are too numerous to show in their entirety. Instead, only a representative sampling of the results is presented. In order to provide greater details of the flow field, only 50 percent of the solution domain is shown in the figures that follow. The effect of angle of attack on the temperature is depicted in Figs. 31a-31d. The temperature profiles in the pitch plane of symmetry are shown in these figures. The following observations can be made from these
Figure 31a. Temperature profiles at $x^*/L^* = 2.5$, $\alpha = 2.5$ deg
Figure 31b. Temperature profiles at \( \frac{x'}{L'} = 2.5, \alpha = 5.0 \text{ deg} \)
Figure 31c. Temperature profiles at $x^*/L^* = 2.5$, $\alpha = 7.5$ deg
Figure 31d. Temperature profiles at $x^*/L^* = 2.5$, $\alpha = 10$ deg
figures: (i) the boundary layer thickens considerably on the leeside while thinning on the windside, (ii) the edge temperatures increase rapidly on the windside while decreasing gradually on the leeside, and (iii) the peak temperatures decrease on the leeside but stay very nearly the same on the windside. The shock on the leeside weakens and begins to smear. At the highest angle of the attack the shock cannot be discerned from the figure. This is due to a combination of central-differencing and coarseness of the grid.

In Figs. 32a-32d, the effect of angle of attack on the mass fraction atomic oxygen in the pitch plane is shown. The amount of atomic oxygen at the wall decreases with increasing angle of attack. However, due to diffusional effects, atomic oxygen is present over a larger distance from the body. On the windside, the amount of atomic oxygen increases at the wall but is present over a smaller distance.

For different angles of attack, the axial variation of the surface pressure and Stanton number on the windward and leeward meridians is shown in Figs. 33a-33d and Figs. 34a-34d, respectively. The increase in surface pressure and heat transfer on the windside and the decrease on the leeside with increasing angle of attack is evident from these figures.

The computations were performed on either the CRAY-XMP/48 or the CRAY-2 (NAS) computers at NASA Ames Research Center. Each test case involved $10 \times 10$ block matrices and required 4.3 milliseconds per grid point per step on the CRAY-XMP computer. The first test case required 2000 steps and the second test case required 1800 steps for the lowest angle of attack calculation to 600 steps for the highest angle of attack calculation.
Figure 32a. $O$ mass fraction profiles at $x^*/L^* = 2.5$, $\alpha = 2.5$ deg
Figure 32b. $O$ mass fraction profiles at $x^*/L^* = 2.5$, $\alpha = 5.0$ deg
Figure 32c. \( O \) mass fraction profiles at \( x^*/L^* = 2.5, \alpha = 7.5 \text{ deg} \)
Figure 32d. $O$ mass fraction profiles at $x^*/L^* = 2.5$, $\alpha = 10$ deg
Figure 33a. Axial variation of surface pressure, $\alpha = 2.5$ deg
Figure 33b. Axial variation of surface pressure, $\alpha = 5.0\ deg$
Figure 33c. Axial variation of surface pressure, $\alpha = 7.5$ deg
Figure 33d. Axial variation of surface pressure, $\alpha = 10 \, deg$
Figure 34a. Axial variation of Stanton number, $\alpha = 2.5 \, \text{deg}$
Figure 34b. Axial variation of Stanton number, $\alpha = 5.0 \text{ deg}$
Figure 34c. Axial variation of Stanton number, $\alpha = 7.5\ deg$
Figure 34d. Axial variation of Stanton number, $\alpha = 10$ deg
CHAPTER 5. CONCLUDING REMARKS

Two new PNS codes have been developed to compute hypersonic laminar flow of chemically reacting air. Temperature variation of species specific heats and enthalpies were taken into account. A noniterative, implicit, space-marching finite-difference method was used to solve the coupled set of gas dynamic and species conservation equations. The conditions for well-posedness of the space-marching method were derived from an eigenvalue analysis of the governing equations. The first code, exclusively for two-dimensional/axisymmetric flow fields, was validated by computing two test cases. These two test cases were, hypersonic flow over a 10 degree wedge and a 10 degree cone at two different altitudes. The computed results were found to be in very good agreement with those of reacting boundary-layer computations. The gas model used in this set of calculations consisted of five species. The species set was later enlarged to include ionized nitric oxide and electrons. The larger species set was employed in the three-dimensional code. This code utilizes a noniterative, implicit, approximately-factored, space-marching method to solve the coupled set of gas dynamic and species conservation equations. In order to validate this code, two test cases were computed. The first test case was that of hypersonic flow over a 10 degree cone at 0 degree angle of attack. The results of this calculation were compared against those of a reacting boundary-layer code. The agreement was found to be very good. These results were further shown to lie between two extremes (ideal gas and equilibrium air). The second test computed was that of hypersonic laminar flow of reacting air over a 10 degree cone at several angles of attack. Due to the unavailability of experimental data for this case, the numerical results were simply compared against the results of the 0 degree
calculation. These calculations were performed not only to demonstrate the three-dimensional capabilities of the code but also to provide "benchmark" calculations for future code developers.

The discontinuities in the flow field are "captured" as part of the solution. Due to the central-differencing employed in the algorithms presented, these discontinuities tend to smear over a few grid points. In order to obtain very crisp shocks, one has two choices, the first is to use upwind differencing based on exact or approximate Riemann solvers, and the second is to "fit" the shock as a sharp discontinuity using Rankine-Hugoniot relations. The former choice has been successfully incorporated into a PNS code for ideal gas/equilibrium air. For the case of finite-rate chemistry, such a procedure gets quite complicated especially if one wants to solve the gas dynamics and chemistry in a coupled manner. The second choice is the easier of the two and therefore, should be pursued further. The scarcity of complete Navier-Stokes solvers to generate starting solutions, limits the use of these new PNS codes to sharp bodies. Currently, an effort is underway to develop a three-dimensional Navier-Stokes code for chemically reacting flow fields. This will increase the scope of using the PNS codes for realistic body shapes.

It is generally recognized that the inclusion of the chemical source terms makes the governing equations "stiff", i.e., the time scales for the gas dynamic and chemistry are disparate. A good measure of the stiffness of a chemically reacting system is the Damköhler number which is the ratio of the fluid dynamic time scale to the chemical time scale. A large value of the Damköhler number implies that the flow is close to equilibrium. In such a situation the stepsizes required to resolve the chemistry become very small. This problem is usually overcome by treating the source terms in an implicit manner. In the present study, the Damköhler numbers
were found to be small implying that the chemical relaxation processes are very slow, \textit{i.e.}, the flow is closer to "frozen" flow. A completely implicit treatment of the chemical source terms was found to have little or no effect on the results presented here. Such a treatment of the chemical source terms will be very important at altitudes lower than those considered in the present study. However, this will lead to substantial increases in both the computational time and memory requirements. Computation of nearly equilibrating flows is being studied currently.

During the writing of this dissertation, a simple turbulence model (Cebeci-Smith) was also incorporated into the code and this option remains to be validated. The present study also indicates that there is a need for a comprehensive experimental database for validation of nonequilibrium codes.
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APPENDIX A. CHEMICAL PRODUCTION TERMS

Consider a multicomponent system of \( n \) species undergoing \( m \) simultaneous elementary reactions. Let \( n_t \) be the total number of reactants. These reactions can be represented symbolically as

\[
\sum_{s=1}^{n_t} \nu_{i,s}^l A_s = \sum_{s=1}^{n_t} \nu_{i,s}'' A_s \quad l = 1, 2, \ldots, m
\]

where \( \nu_{i,s}^l, \nu_{i,s}'' \) are the stoichiometric coefficients and \( A_s \) is the chemical symbol of the \( s \)th species. Using the law of mass action, the nondimensional mass production rate of species \( s \) is

\[
\dot{w}_s = M_s \sum_{l=1}^{m} (\nu_{i,s}'' - \nu_{i,s}^l) \left\{ k_{f,l}(T) \prod_{r=1}^{n_t} [\rho r \gamma_r \nu_{i,r}^l - k_{b,l}(T) \prod_{r=1}^{n_t} [\rho r \gamma_r \nu_{i,r}''] \right\}
\]

(A1)

The nondimensional mole-mass ratios of the reactants are defined as

\[
\gamma_r = \begin{cases} 
\frac{c_r}{M_r} & \text{for } r = 1, 2, \ldots, n \\
\sum_{s=1}^{n} z_{(r-n),s} \gamma_s & \text{for } r = n + 1, n + 2, \ldots, n_t 
\end{cases}
\]

(A2)

The reaction rates are functions of temperature and are expressed in the modified Arrhenius form, i.e., the nondimensional forward and backward rates are written as

\[
k_{f,l}(T) = \exp(\log_c C'_{1,l} + \frac{C'_{2,l}}{T} + C'_{3,l} \log T) \quad \text{(A3)}
\]

\[
k_{b,l}(T) = \exp(\log_c D'_{1,l} + \frac{D'_{2,l}}{T} + D'_{3,l} \log T) \quad \text{(A4)}
\]

where

\[
C'_{1,l} = \frac{L}{V_{\infty}} \left( \frac{\rho_{\infty}}{M_{\infty}} \right)^{\alpha l - 1} 10^{3-3\alpha l} T_{\infty}^{C'_{2,l}} C_{1,l}, \quad C'_{2,l} = \frac{C'_{2,l}}{T_{\infty}} \quad \text{(A5)}
\]

\[
D'_{1,l} = \frac{L}{V_{\infty}} \left( \frac{\rho_{\infty}}{M_{\infty}} \right)^{\beta l - 1} 10^{3-3\beta l} T_{\infty}^{D'_{2,l}} D_{1,l}, \quad D'_{2,l} = \frac{D'_{2,l}}{T_{\infty}} \quad \text{(A6)}
\]

\[
\alpha_l = \sum_{r=1}^{n_t} \nu_{i,r}, \quad \beta_l = \sum_{r=1}^{n_t} \nu_{i,r}''
\]

(A7)

and \( C_{1,l}, C_{2,l}, C_{3,l}, D_{1,l}, D_{2,l}, \) and \( D_{3,l} \) are constants for a particular reaction \( l \).
APPENDIX B. ANALYSIS OF PNS EQUATIONS

The influence of the streamwise pressure gradient on the mathematical character of the PNS equations is studied in this section. For simplicity, planar two-dimensional flow of a binary mixture is considered. Further, the coordinate transformation is assumed to be the identity map, i.e., $\xi=x$ and $\eta=y$. There is no loss of generality in doing so.

The speed of sound required in the analysis is defined [40] as

$$a_f^2 = -\frac{\partial h}{\partial \rho}_{\rho_c}\left(\frac{\partial h}{\partial \rho}_{\rho_c} - \frac{1}{\rho}\right)^{-1}$$

(B1)

where the subscripts on the derivatives denote the quantities that are held constant during the differentiation. Using the equation of state and the definition of the frozen specific heat, Eq. B1 can be rewritten as

$$a_f^2 = \beta_1 C_{pf} T \left(M C_{pf} - \beta_1 \right)^{-1} = \frac{\psi}{(1 - \chi)}$$

(B2)

where

$$\chi = \frac{\beta_1}{MC_{pf}}, \quad \psi = \frac{\beta_1 T}{M}$$

(B3)

Following Vigneron et al. [34], only a fraction $\omega (0 \leq \omega \leq 1)$ of the streamwise pressure gradient is retained. First, consider the inviscid limit ($Re \to \infty$) of the PNS equations. The equations can be written in nonconservation-law form as

$$A^i Q_x + B^i Q_y = W^c$$

(B4)

where

$$Q = (\rho, u, v, h, c_1)^T, \quad W^c = (0, 0, 0, 0, \dot{\psi}_1)^T$$

(B5)
\[
A^i = \begin{pmatrix}
u & \rho & 0 & 0 & 0 \\
\omega \psi & \rho u & 0 & \rho \omega \chi & \omega \phi \\
0 & 0 & \rho u & 0 & 0 \\
0 & \rho u^2 & \rho uv & \rho u & 0 \\
0 & 0 & 0 & 0 & \rho u
\end{pmatrix}
\]

\[
B^i = \begin{pmatrix}
u & 0 & \rho & 0 & 0 \\
0 & \rho v & 0 & 0 & 0 \\
\phi & \rho v & \rho \chi & \phi \\
0 & \rho uv & \rho v^2 & \rho v & 0 \\
0 & 0 & 0 & 0 & \rho v
\end{pmatrix}
\]

\[
\phi = \rho \psi M \left( \frac{1}{M_1} - \frac{1}{M_2} \right) - \rho \chi (h_1 - h_2)
\]

The pressure has been eliminated from the PNS equations using the following expression

\[
\frac{\partial \rho}{\partial \alpha} = \psi \frac{\partial \rho}{\partial \alpha} + \rho \chi \frac{\partial h}{\partial \alpha} + \beta_1 \rho \sum_{s=1}^{n} \left( \frac{T}{M_s} - \frac{h_s}{MC_p} \right) \frac{\partial c_s}{\partial \alpha} \quad \alpha = x, y
\]

The system of equations is hyperbolic in the \( x \)-direction if the eigenvalues of \((A^i)^{-1}(B^i)\) are real. These eigenvalues are

\[
\lambda_{1,2,3} = \frac{v}{u}, \quad \lambda_{4,5} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}
\]

where

\[
a = u^2(1 - \omega \chi) - \omega \psi \\
b = -uv \left[ 2 - \chi(1 + \omega) \right] \\
c = v^2(1 - \chi) - \psi
\]

If the streamwise pressure gradient term is completely retained, i.e., \( \omega = 1 \), then it can be shown that the eigenvalues are real if

\[
u^2 + v^2 \geq \frac{\psi}{(1 - \chi)} = a_f^2
\]

or

\[
M_f^2 \geq 1
\]
where $M_f$ is the frozen Mach number. On the other hand, if only a fraction of the pressure gradient is retained, i.e., $0 \leq \omega < 1$, the eigenvalues will remain real in the subsonic part of the flow if

$$\omega \leq M C_{p_f} u^2 \left( \beta_1 C_{p_f} T + \beta_1 u^2 \right)^{-1} \tag{B13}$$

where $v$ is assumed to be negligibly small compared to $u$.

Next, consider the viscous limit of the PNS equations and neglect the first derivatives in $y$. Assuming that the transport properties are locally constant, the system of equations can be written as

$$A^i Q_x = M^\nu Q_{yy} + W^c \tag{B14}$$

where

$$M^\nu = \frac{\mu}{Re} \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & \frac{4}{3} & 0 & 0 \\
0 & u & \frac{4}{3} u & \frac{1}{Pr_f} & \frac{C_p-1}{Pr_f} (h_1 - h_2) \\
0 & 0 & 0 & 0 & \frac{C_p}{Pr_f}
\end{pmatrix} \tag{B15}$$

The temperature gradient in the $y$-direction has been replaced by

$$\frac{\partial T}{\partial y} = \frac{1}{C_{p_f}} \left\{ \frac{\partial h}{\partial y} - \sum_{s=1}^{n} \frac{h_s}{C_s} \right\} \tag{B16}$$

The system is parabolic in the positive $x$-direction if and only if the eigenvalues of $(A^i)^{-1}(M^\nu)$ are real and positive. Assuming that $u$ is nonzero, these eigenvalues are obtained from the following equation
It can be shown that the eigenvalues obtained from this equation are real and positive if

\[ u > 0 \]  \hspace{1cm} (B18)

\[ \omega < M C_p T \left( \beta_1 C_p T + \beta_1 u^2 \right)^{-1} \]  \hspace{1cm} (B19)

It is easily seen from Eq. B18, Eq. B12, and Eq. B13 that the space-marching method is well-posed if and only if (i) there is no axial flow separation, (ii) the frozen Mach number in the inviscid part of the flow field is greater than 1, and (iii) only a fraction of the streamwise pressure gradient is retained in subsonic part of the flow field. Alternately, conditions (ii) and (iii) can be combined and stated as the following condition; the streamwise pressure gradient term is completely retained if the streamwise frozen Mach number is greater than unity, otherwise only a fraction of it is retained.

For an ideal (nonreacting) gas with constant specific heats the expression for \( \omega \) reduces to the familiar Vigneron condition [34]. This is easily seen by substituting the following into Eq. B12

\[ \beta_1 = \frac{1}{\gamma M_{\infty}^2}, \quad C_{p_f} = \frac{1}{(\gamma - 1) M_{\infty}^2}, \quad u^2 = \frac{M_z^2 T}{M_{\infty}^2}, \quad M = 1 \]  \hspace{1cm} (B20)

to obtain the condition

\[ \omega \leq \gamma M_z^2 \left[ 1 + (\gamma - 1) M_z^2 \right]^{-1} \]  \hspace{1cm} (B21)
APPENDIX C. INVISCID JACOBIANS

The inviscid Jacobian represents the linearization of the inviscid fluxes. When the gas dynamic equations are coupled with the chemistry equations, the Jacobian is an \((n + 4) \times (n + 4)\) matrix where \(n\) is the number of species. In what follows, expressions for the matrix elements of the three-dimensional inviscid Jacobian matrices are derived.

The vector of dependent variables is repeated here for the sake of clarity

\[
Q = \{\rho, \rho u, \rho v, \rho w, \rho H, \rho e_1, c_2, \ldots, \rho e_{n-1}\}^T = \{Q^1, Q^2, \ldots, Q^{n+4}\}^T \tag{C1}
\]

In the linearization of the fluxes, expressions for \(\partial p/\partial Q\) are required. These expressions are obtained in the following manner. The specific static enthalpy of the mixture is by definition

\[
h = \sum_{j=1}^{n} c_j h_j(T) \tag{C2}
\]

Differentiating both sides of Eq. C2 with respect to \(Q^k\) (\(Q^k\) is the \(k\)th element of the vector \(Q\)) one has

\[
\frac{\partial h}{\partial Q^k} = \sum_{j=1}^{n} c_j \frac{\partial}{\partial Q^k} [h_j(T)] + \sum_{j=1}^{n} h_j(T) \frac{\partial c_j}{\partial Q^k} \tag{C3}
\]

Noting that the species enthalpy is a function of temperature alone and using the definition of specific heat, Eq. C3 can be rewritten as

\[
\frac{\partial h}{\partial Q^k} = \left(\sum_{j=1}^{n} c_j C_{p_j}\right) \frac{\partial T}{\partial Q^k} + \sum_{j=1}^{n} h_j(T) \frac{\partial c_j}{\partial Q^k} = C_{p_f} \frac{\partial T}{\partial Q^k} + \sum_{j=1}^{n} h_j(T) \frac{\partial c_j}{\partial Q^k} \tag{C4}
\]

Rearranging terms in Eq. C4 and using the definition of total enthalpy of the mixture, the final expression for \(\partial T/\partial Q^k\) is

\[
\frac{\partial T}{\partial Q^k} = \frac{1}{C_{p_f}} \left[ \frac{\partial H}{\partial Q^k} - \frac{1}{2} \frac{\partial V^2}{\partial Q^k} - \sum_{j=1}^{n} h_j(T) \frac{\partial c_j}{\partial Q^k} \right] \tag{C5}
\]
Now the equation of state for the mixture, Eq. 4, is

\[ p = \frac{\beta_1 \rho T}{M} = \beta_1 T \sum_{j=1}^{n} \frac{\rho c_i}{M_j} \]  

(C6)

Differentiating both sides of Eq. C6 with respect to \( Q^k \) one has

\[ \frac{\partial p}{\partial Q^k} = \beta_1 T \sum_{j=1}^{n} \frac{\partial}{\partial Q^k} \left( \frac{\rho c_i}{M_j} \right) + \frac{\beta_1 \rho}{M} \frac{\partial T}{\partial Q^k} \]  

(C7)

Substituting Eq. C5 into Eq. C7, the final expression for \( \partial p/\partial Q^k \) is

\[ \frac{\partial p}{\partial Q^k} = \beta_1 T \sum_{j=1}^{n} \frac{\partial}{\partial Q^k} \left( \frac{\rho c_i}{M_j} \right) + \frac{\beta_1 \rho}{M C_{pf}} \left[ \frac{\partial H}{\partial Q^k} - \frac{1}{2} \frac{\partial V^2}{\partial Q^k} - \sum_{j=1}^{n} h_j(T) \frac{\partial c_j}{\partial Q^k} \right] \]  

(C8)

Define the following quantities

\[ \phi_s = \begin{cases} 
MC_{pf} T(1/M_s - 1/M_n) - (h_s - h_n) & \text{if } s < n; \\
MC_{pf} T(1/M_n) - h_n & \text{if } s = n. 
\end{cases} \]  

(C9)

\[ \chi = \frac{\beta_1}{MC_{pf}} \]  

(C10)

Using Eqs. C8, C9, and C10, the elements of the vector \( \partial p/\partial Q \) are

\[ \begin{align*}
\frac{\partial p}{\partial Q^1} &= \chi \left( \frac{V^2}{2} + \phi_n \right) \\
\frac{\partial p}{\partial Q^2} &= -\chi u \\
\frac{\partial p}{\partial Q^3} &= -\chi v \\
\frac{\partial p}{\partial Q^4} &= -\chi w \\
\frac{\partial p}{\partial Q^5} &= \chi \\
\frac{\partial p}{\partial Q^6} &= \chi \phi_1 \\
\frac{\partial p}{\partial Q^7} &= \chi \phi_2 \\
&\quad \vdots \\
\frac{\partial p}{\partial Q^{n+4}} &= \chi \phi_{n-1} 
\end{align*} \]  

(C11)

The elements of the inviscid Jacobian matrix are derived next. First consider the generalized global mass flux. This flux can be written as

\[ E_1^i = \frac{1}{J} (S_x \rho u + S_y \rho v + S_z \rho w) = \rho \hat{U} \]  

\[ = \hat{S}_x Q^2 + \hat{S}_y Q^3 + \hat{S}_z Q^4 \]  

(C12)
where $S_x$, $S_y$, $S_z$, and $J$ are the metrics and Jacobian of the coordinate transformation and

$$
\hat{U} = \hat{S}_x u + \hat{S}_y v + \hat{S}_z w \quad (C13)
$$

$$
\hat{S}_x = \frac{S_x}{J}, \quad \hat{S}_y = \frac{S_y}{J}, \quad \hat{S}_z = \frac{S_z}{J} \quad (C14)
$$

Differentiating Eq. C12 with respect to the elements of $Q$, the elements of the first row of the inviscid Jacobian matrix are obtained. The elements of this row are

$$
\hat{A}_{1,2} = \hat{S}_x \\
\hat{A}_{1,3} = \hat{S}_y \\
\hat{A}_{1,4} = \hat{S}_z
$$

Next consider the generalized momentum flux in the $\xi$ direction. This flux can be written as

$$
E_2^i = \frac{1}{J} (S_x u^2 + S_y u v + S_z u w + \omega S_z p) \\
= \hat{S}_x \frac{Q^2 Q^2}{Q^1} + \hat{S}_y \frac{Q^2 Q^3}{Q^1} + \hat{S}_z \frac{Q^2 Q^4}{Q^1} + \omega \hat{S}_z p \quad (C16)
$$

Differentiating Eq. C16 with respect to the elements of $Q$ and using Eq. C12, the elements of the second row of the inviscid Jacobian matrix are obtained. The elements of this row are

$$
\hat{A}_{2,1} = -u\hat{U} + \omega \hat{S}_z (\frac{V^2}{2} + \phi_n) \\
\hat{A}_{2,2} = (1 - \omega \chi) \hat{S}_z u + \hat{U} \\
\hat{A}_{2,3} = \hat{S}_y u - \omega \chi \hat{S}_z v \\
\hat{A}_{2,4} = \hat{S}_z u - \omega \chi \hat{S}_z w \\
\hat{A}_{2,5} = \omega \chi \hat{S}_z \\
\hat{A}_{2,6} = \omega \chi \hat{S}_z \phi_1 \\
\hat{A}_{2,7} = \omega \chi \hat{S}_z \phi_2 \\
\vdots \\
\hat{A}_{2,n+4} = \omega \chi \hat{S}_z \phi_{n-1}
$$

(C17)
The elements of the third and fourth rows of the inviscid Jacobian matrix correspond to the generalized momentum fluxes in the \( \eta \) and \( \zeta \) directions, respectively and are obtained in a manner similar to that shown above. The elements of these rows are

\[
\begin{align*}
\hat{A}_{3,1} &= -v\hat{U} + \omega \chi \hat{S}_y \left( \frac{V^2}{2} + \phi_n \right) \\
\hat{A}_{3,2} &= \hat{S}_z v - \omega \chi \hat{S}_y u \\
\hat{A}_{3,3} &= (1 - \omega \chi) \hat{S}_y v + \hat{U} \\
\hat{A}_{3,4} &= \hat{S}_z v - \omega \chi \hat{S}_y w \\
\hat{A}_{3,5} &= \omega \chi \hat{S}_y \\
\hat{A}_{3,6} &= \hat{S}_y \phi_1 \\
\hat{A}_{3,7} &= \omega \chi \hat{S}_y \phi_2 \\
&\vdots \\
\end{align*}
\]

\begin{align*}
\hat{A}_{4,1} &= -w\hat{U} + \omega \chi \hat{S}_z \left( \frac{V^2}{2} + \phi_n \right) \\
\hat{A}_{4,2} &= \hat{S}_z w - \omega \chi \hat{S}_z u \\
\hat{A}_{4,3} &= \hat{S}_y w - \omega \chi \hat{S}_z v \\
\hat{A}_{4,4} &= (1 - \omega \chi) \hat{S}_z w + \hat{U} \\
\hat{A}_{4,5} &= \omega \chi \hat{S}_z \\
\hat{A}_{4,6} &= \hat{S}_z \phi_1 \\
\hat{A}_{4,7} &= \omega \chi \hat{S}_z \phi_2 \\
&\vdots \\
\hat{A}_{4,n+4} &= \omega \chi \hat{S}_z \phi_{n-1}
\end{align*}

(C18)

The generalized energy flux can be written as

\[
E^i_5 = \frac{1}{J} \left( S_x \rho u H + S_y \rho v H + S_z \rho w H \right)
\]

\[
= \hat{S}_z \frac{Q^2 Q^5}{Q^1} + \hat{S}_y \frac{Q^3 Q^5}{Q^1} + \hat{S}_z \frac{Q^4 Q^5}{Q^1}
\]

(C20)

Differentiating Eq. C20 with respect to the elements of \( \mathbf{Q} \), the elements of the fifth row of the inviscid Jacobian matrix are obtained. The elements of this row are

\[
\begin{align*}
\hat{A}_{5,1} &= -\hat{U} H \\
\hat{A}_{5,2} &= \hat{S}_z H \\
\hat{A}_{5,3} &= \hat{S}_y H \\
\hat{A}_{5,4} &= \hat{S}_z H \\
\hat{A}_{5,5} &= \hat{U} 
\end{align*}
\]

(C21)
The generalized mass flux of species \( s \) (\( s = 1, 2, \ldots, n - 1 \)) can be written as

\[
E_{5+s}^i = \frac{1}{f} (S_x p u c_s + S_y p v c_s + S_z p w c_s)
\]

\[
= \hat{S}_x \frac{Q^2 Q^{5+s}}{Q^1} + \hat{S}_y \frac{Q^2 Q^{5+s}}{Q^1} + \hat{S}_z \frac{Q^4 Q^{5+s}}{Q^1}
\]  \hspace{1cm} (C22)

Differentiating Eq. C22 with respect to the elements of \( Q \), the elements of the \((5+s)\)th row of the inviscid Jacobian matrix are obtained. The elements of this row are

\[
\hat{A}_{5+s,1} = -\hat{U} c_s
\]

\[
\hat{A}_{5+s,2} = \hat{S}_x c_s
\]

\[
\hat{A}_{5+s,3} = \hat{S}_y c_s
\]  \hspace{1cm} (C23)

\[
\hat{A}_{5+s,4} = \hat{S}_z c_s
\]

\[
\hat{A}_{5+s,5+s} = \hat{U}
\]

The elements not listed in the preceding derivations are identically zero. The elements of the inviscid Jacobian \( \partial \hat{E}^i / \partial Q \) are obtained by substituting \( \xi \) for the symbol \( S \). The elements of the inviscid Jacobian \( \partial \hat{G}^i / \partial Q \) (\( \partial \hat{G}^i / \partial Q \)) are obtained by (i) substituting \( \eta \) (\( \zeta \)) for the symbol \( S \) and (ii) setting \( \omega = 1 \).
APPENDIX D. VISCOUS JACOBIAN

The viscous Jacobian is also an \((n + 4) \times (n + 4)\) matrix. The expressions for the elements of this matrix are derived in this section. The following notation is used

\[
\psi_s = J \ell_s \quad s = 1, 2, \ldots, n + 7
\]  

\((D1)\)

where \(\ell_1, \ell_2, \ldots, \ell_{n+7}\) are defined in Eq. 13.

The generalized viscous momentum flux in the \(\xi\) direction, is written as

\[
F_2^\nu = \psi_1 u_\eta + \psi_4 v_\eta + \psi_5 w_\eta
= \psi_1 \left( \frac{Q^2}{Q^1} \right)_\eta + \psi_4 \left( \frac{Q^3}{Q^1} \right)_\eta + \psi_5 \left( \frac{Q^4}{Q^1} \right)_\eta
\]  

\((D2)\)

Differentiating Eq. \(D2\) with respect to the elements of \(Q\), the elements of the second row of the viscous Jacobian matrix are

\[
\dot{M}_{2,1} = -\left[ \psi_1 \left( \frac{u}{\rho} \right)_\eta + \psi_4 \left( \frac{v}{\rho} \right)_\eta + \psi_5 \left( \frac{w}{\rho} \right)_\eta \right]
\]

\[
\dot{M}_{2,2} = \psi_1 \left( \frac{1}{\rho} \right)_\eta
\]

\[
\dot{M}_{2,3} = \psi_4 \left( \frac{1}{\rho} \right)_\eta
\]

\[
\dot{M}_{2,4} = \psi_5 \left( \frac{1}{\rho} \right)_\eta
\]  

\((D3)\)

The elements of the third and fourth rows are obtained in a similar manner by considering the generalized viscous momentum fluxes in the \(\eta\) and \(\zeta\) directions. The elements of these rows are

\[
\dot{M}_{3,1} = -\left[ \psi_4 \left( \frac{u}{\rho} \right)_\eta + \psi_2 \left( \frac{v}{\rho} \right)_\eta + \psi_3 \left( \frac{w}{\rho} \right)_\eta \right]
\]

\[
\dot{M}_{3,2} = \psi_4 \left( \frac{1}{\rho} \right)_\eta
\]

\[
\dot{M}_{3,3} = \psi_2 \left( \frac{1}{\rho} \right)_\eta
\]

\[
\dot{M}_{3,4} = \psi_3 \left( \frac{1}{\rho} \right)_\eta
\]  

\((D4)\)
The generalized viscous energy flux is written as

\[ F_5 = \frac{1}{2} (\psi_1 - \psi_7) (u^2)_n + \frac{1}{2} (\psi_2 - \psi_8) (v^2)_n + \frac{1}{2} (\psi_3 - \psi_8) (w^2)_n + \psi_4 (uv)_n + \psi_5 (uw)_n + \psi_6 (vw)_n + \psi_7 H_n + \psi_9 (c_1)_n + \psi_{10} (c_2)_n + \ldots + \psi_{n+7} (c_{n-1})_n \]

Differentiating Eq. D6 with respect to the elements of the vector \( Q \), the elements of the fifth row of the viscous Jacobian matrix are obtained. The elements of this row are

\[ \dot{M}_{5,1} = - [(\psi_1 - \psi_7) (u^2)_n + (\psi_2 - \psi_7) (v^2)_n + (\psi_3 - \psi_7) (w^2)_n + 2 \psi_4 (uv)_n + 2 \psi_5 (uw)_n + 2 \psi_6 (vw)_n + \psi_7 (H)_n + \psi_9 (c_1)_n + \psi_{10} (c_2)_n + \ldots + \psi_{n+7} (c_{n-1})_n] \]

\[ \dot{M}_{5,2} = (\psi_1 - \psi_7) (\frac{u}{\rho})_n + \psi_4 (\frac{v}{\rho})_n + \psi_5 (\frac{w}{\rho})_n \]

\[ \dot{M}_{5,3} = \psi_4 (\frac{u}{\rho})_n + (\psi_2 - \psi_7) (\frac{v}{\rho})_n + \psi_6 (\frac{w}{\rho})_n \]

\[ \dot{M}_{5,4} = \psi_5 (\frac{u}{\rho})_n + \psi_6 (\frac{v}{\rho})_n + (\psi_3 - \psi_7) (\frac{w}{\rho})_n \]
Finally, the generalized diffusion mass flux of species $s$ ($s = 1, 2, \ldots, n - 1$) is written as

$$F_5^{s+s} = \psi_8(\frac{c_s}{\rho})_\eta$$

$$= \psi_8(\frac{Q^{s+s}}{Q^1})_\eta$$

(D8)

The elements of the $(s + 5)$th row of the viscous Jacobian matrix are obtained by differentiating Eq. D8 with respect to the elements of $Q$. These elements are

$$\dot{M}_{s+5,1} = -\psi_8(\frac{c_s}{\rho})_\eta$$

$$\dot{M}_{s+5,5+s} = \psi_8(\frac{1}{\rho})_\eta$$

(D9)

The elements not listed are identically zero and the subscript $\eta$ denotes the partial derivative with respect to $\eta$. 
APPENDIX E. SOURCE TERM JACOBIAN

The chemical source vector, $\mathbf{W}^c$, is a function of the mixture temperature, density, and mass concentrations. This is mathematically expressed as

$$\mathbf{W}^c = \frac{1}{J} \mathbf{w}^c(T, \rho \gamma_1, \rho \gamma_2, \ldots, \rho \gamma_n)$$  \hspace{1cm} (E1)

The Jacobian of the source term is

$$\mathbf{J}^c = \frac{\partial \mathbf{W}^c}{\partial \mathbf{Q}} = \frac{1}{J} \frac{\partial \mathbf{W}^c}{\partial \mathbf{Q}}$$  \hspace{1cm} (E2)

Using Eq. E1 and the chain rule, the partial derivative in Eq. E2 can be written as

$$\frac{\partial \mathbf{W}^c}{\partial \mathbf{Q}} = \frac{\partial \mathbf{W}^c}{\partial T} \frac{\partial T}{\partial \mathbf{Q}} + \frac{\partial \mathbf{W}^c}{\partial \Gamma} \frac{\partial \Gamma}{\partial \mathbf{Q}}$$  \hspace{1cm} (E3)

where

$$\Gamma = \{\rho \gamma_1, \rho \gamma_2, \ldots, \rho \gamma_n\}^T$$  \hspace{1cm} (E4)

The derivative $\partial \mathbf{W}^c / \partial T \quad [(n + 4) \times 1 \text{ column vector}]$ is easily evaluated since the reaction rate constants are the only quantities that depend explicitly on the temperature. The derivative $\partial T / \partial \mathbf{Q}$ is a $1 \times (n + 4)$ row vector whose elements are

$$\frac{\partial T}{\partial \mathbf{Q}} = \frac{1}{\rho C_p} \left\{ \frac{V^2}{2} - h_n, -u, -v, -w, 1, -(h_1 - h_n), \ldots, -(h_{n-1} - h_n) \right\}$$  \hspace{1cm} (E5)

Evaluation of the second term of Eq. E3 is little more involved. The derivative $\partial \mathbf{W}^c / \partial \Gamma \quad [(n + 4) \times n_t \text{ matrix}]$ is obtained by differentiating Eq. A1 with respect to the elements of $\Gamma$. This process is cumbersome especially when the number of elementary reactions is large. The derivative $\partial \Gamma / \partial \mathbf{Q} \quad [n_t \times (n + 4) \text{ matrix}]$ is easily evaluated using Eq. A2.