Computation of Three-Dimensional Chemically Reacting Viscous Flow around Rocket Body

By

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Summary: A hybrid scheme that treats the strong peripheral shock as sharp shock is developed to compute the hypersonic, viscous and chemically reacting three-dimensional flow around a rocket body. A multi-component mixture of thermally perfect but calorically imperfect gas is used. Diffusion velocities at all grid points are computed by solving multi-component diffusion equations. All the molecular diffusion transport terms are retained. The governing equations in conservation-law form are solved using a non-iterative, approximately-factored implicit finite-difference scheme. Both fully-catalytic and non-catalytic walls are treated. Laminar flowfields over a rocket nose configuration are generated for different gas models and boundary conditions.

NOMENCLATURE

$\hat{A}, \hat{B}, \hat{C}$	: inviscid Jacobian matrices	Pr	: Prandtl number
c_f	: skin-friction coefficient	$\hat{q}$	: conservational variables vector
c_p	: pressure coefficient	q	: heat transfer rate
C	: molar concentration	Q_D	: diffusion heat transfer rate
D	: binary diffusion coefficient	R_0	: universal gas constant
e	: internal energy	Re	: Reynolds number
$\hat{E}, \hat{F}, \hat{G}$	: inviscid flux vectors	s	: distance along the body
$\hat{E}_v, \hat{F}_v, \hat{G}_v$	: viscous flux vectors	Sn	: Stanton number
f	: mass fraction	t	: time coordinate
h	: static enthalpy	T	: temperature
h_f^0	: enthalpy of formation at reference temperature T_f^0	T_e	: effective temperature
H	: total enthalpy	T_0, T'_0	: Sutherland's constants
k_f	: forward reaction-rate constant	T_f^0	: reference temperature, 298.0K
k_b	: backward reaction-rate constant	u, v, w	: Cartesian velocity components
K_c	: equilibrium constant	U, V, W	: contravariant velocities
L^*	: reference length=1 m	$\tilde{u}, \tilde{v}, \tilde{w}$	: diffusion velocities in Cartesian coordinates
Le	: Lewis number	$\tilde{V}_n$	: diffusion velocity in the direction normal to body
M	: molecular mass	V_∞	: freestream velocity
M	: third body	$\dot{W}$	: mass production rate
M_f	: freestream Mach number	x, y, z	: Cartesian coordinates
N_s	: number of species in the mixture	X	: molar fraction
N_r	: number of reactions involved		
p	: static pressure		

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Greek letter symbols

α	: angle of attack
Ω_0	: diffusion collision integral
κ	: thermal conductivity
κ_0	: Sutherland's constant
μ	: viscosity
μ_0	: Sutherland's constant
ν'	: stoichiometric coefficient for species appearing as reactant
ν''	: stoichiometric coefficient for species appearing as product
ξ, η, ζ	: general body-oriented coordinates
ρ	: density
σ	: effective collision diameter

Subscripts

i, j	: indices denoting species
w	: wall
x, y, z	: partial derivatives with respect to x, y, z
ξ, η, ζ	: partial derivatives with respect to ξ , η, ζ
∞	: freestream

Superscripts

*	: dimensional variables
n	: n-th level in time

INTRODUCTION

Computation of non-equilibrium flows received considerable attention in 1960's and early 1970's. During that period due to inadequate computing facilities and narrower domain of applications, most of calculations [1] were made on coarse meshes; they were not sufficient to describe rapidly changing species concentrations, giving only macroscopic solutions. In late 70's powerful techniques to generate meshes around complicated geometries, and to reproduce ideal gas flows associated with any flying body were developed by keeping pace with miraculous advancement in computer hardware technology. In recent years, advent of supercomputers, which have super memories and can calculate at super speeds, has challenged numerical fluid dynamicists and lead many researchers to compute flowfields around a complete flying vehicle configuration. On the other hand, new space projects such as space transport vehicles and orbital transport vehicles, demand enhancement in the capability of these vehicles which choose considerably high altitude flight trajectories within the atmosphere. When a vehicle is traveling at a hypersonic velocity at a high altitude where the air density is low, the flow behind the bow shock wave formed over the vehicle will tend to be chemically and thermodynamically out of equilibrium. In the non-equilibrium regime of a flow, the thermal energy of the gas will be higher than its equilibrium value because the absorption of energy due to dissociation does not take place to the extent dictated by the equilibrium conditions. Park [2] has recently made a preliminary study of the thermally and chemically non-equilibrium shock-layer in a simulation of one-dimensional shock tube flow with a time dependent implicit method, and Lee [3] has proposed a set of basic governing equations to describe these flows. Extension of these analyses to higher dimensional flows is quite complicated and requires further research. However, the problem can be simplified by assuming the flowfield to be in thermally equilibrium but not in chemically equilibrium. Especially when ionization is not significant, the one temperature model is sufficient to describe the flow.

The numerical methods currently available to solve viscous and chemically reacting

flows around three-dimensional bodies can be broadly categorized into shock capturing and shock fitting schemes. The schemes which use viscous shock layer (VSL) [4] equations fall into the latter category and are widely used by a number of authors [5, 6]. The non-conservation form of VSL equations is uniformly valid in the shock layer but fails in the presence of crossflow separation and of course in the presence of any internal shocks. In the former category, the methods which use Parabolized Navier-Stokes (PNS) [7] equations are becoming popular because of their shorter computation time. However, in these space marching procedures, additional restrictions are placed on the stream-wise convective terms which invalidate these schemes in the presence of any axial flow separation and in general are invalid in the subsonic inviscid flow regime. On the other hand, use of time-dependent conservation equations to solve a steady-state problem circumvents all these problems but requires a substantial amount of computation time. Efficiency of those schemes can be improved appreciably by fitting amenable shocks such as a peripheral shock and capturing all the other weak internal shocks. Such techniques are proven efficient in finite volume formulation in the past by Rizzi [9] and recently by Gnoffo [10]. Since the introduction of Beam-Warming implicit scheme [11], ideal gas flowfields over complicated bodies are reproduced quite accurately. Being implicit in nature, this scheme is quite stable even in the presence of severe stiffness problems associated with chemical reactions. Realizing that this scheme will offer a powerful tool in computing chemically reacting flows, a hybrid technique for Beam-Warming scheme that fits a peripheral bow shock as sharp shock and captures all the other internal shocks is developed in the present study.

The present paper describes in detail the development of this new hybrid Beam-Warming scheme that can compute chemically reacting three-dimensional flowfields around a rocket body. The gas medium considered is air consisting of five chemical species that are involved in five chemical reactions. The conventional gasdynamic equations along with the species conservation equations are solved simultaneously using a non-iterative, implicit and approximately-factored Beam-Warming finite-difference method. At each time step the species diffusion velocities are computed by solving the multi-component diffusion equations. The numerical results obtained for two-dimensional and axi-symmetric sphere-cone rocket nose configurations at angles of attack at various flight speeds are presented.

MATHEMATICAL MODEL

Governing Equations:

A complete system of governing equations that describe a three-dimensional, viscous flow of a multi-component reacting gas is obtained from Reference 12, (i) after assuming the flow to be in thermal equilibrium, (ii) neglecting radiation and body forces and (iii) assuming mass diffusion to be binary only. These equations in a general moving curvilinear coordinate system (ξ , η , ζ and τ) can be rewritten in a strong conservation-law form after introducing non-dimensional variables as follows:

$$\frac{\partial \hat{q}}{\partial \tau} + \frac{\partial \hat{E}}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} + \frac{\partial \hat{G}}{\partial \zeta} = \frac{1}{\text{Re}} \left[\frac{\partial \hat{E}_v}{\partial \xi} + \frac{\partial \hat{F}_v}{\partial \eta} + \frac{\partial \hat{G}_v}{\partial \zeta} \right] + \hat{H}, \quad (1)$$

where the (N_s+4) component inviscid fluxes are

$$\hat{q} = J^{-1} \begin{pmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho w \\ e \end{pmatrix}, \quad \hat{E} = J^{-1} \begin{pmatrix} \rho_i U \\ \rho u U + \xi_x p \\ \rho v U + \xi_y p \\ \rho w U + \xi_z p \\ (e+p)U - \xi_i p \end{pmatrix},$$

$$\hat{F} = J^{-1} \begin{pmatrix} \rho_i V \\ \rho u V + \eta_x p \\ \rho v V + \eta_y p \\ \rho w V + \eta_z p \\ (e+p)V - \eta_i p \end{pmatrix}, \quad \hat{G} = J^{-1} \begin{pmatrix} \rho_i W \\ \rho u W + \zeta_x p \\ \rho v W + \zeta_y p \\ \rho w W + \zeta_z p \\ (e+p)W - \zeta_i p \end{pmatrix},$$

with

$$U = \xi_t + \xi_x u + \xi_y v + \xi_z w,$$

$$V = \eta_t + \eta_x u + \eta_y v + \eta_z w,$$

$$W = \zeta_t + \zeta_x u + \zeta_y v + \zeta_z w.$$

Here U , V , and W are the contravariant velocities.

The (N_s+4) component viscous and molecular diffusion fluxes in Eq. (1) are as follows:

$$\hat{E}_v = J^{-1} \begin{pmatrix} -\rho_i \beta_3 (\xi_x \tilde{u}_i + \xi_y \tilde{v}_i + \xi_z \tilde{w}_i) \\ \xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz} \\ \xi_x \tau_{yx} + \xi_y \tau_{yy} + \xi_z \tau_{yz} \\ \xi_x \tau_{zx} + \xi_y \tau_{zy} + \xi_z \tau_{zz} \\ \xi_x \beta_x + \xi_y \beta_y + \xi_z \beta_z \end{pmatrix}, \quad \hat{F}_v = J^{-1} \begin{pmatrix} -\rho_i \beta_3 (\eta_x \tilde{u}_i + \eta_y \tilde{v}_i + \eta_z \tilde{w}_i) \\ \eta_x \tau_{xx} + \eta_y \tau_{xy} + \eta_z \tau_{xz} \\ \eta_x \tau_{yx} + \eta_y \tau_{yy} + \eta_z \tau_{yz} \\ \eta_x \tau_{zx} + \eta_y \tau_{zy} + \eta_z \tau_{zz} \\ \eta_x \beta_x + \eta_y \beta_y + \eta_z \beta_z \end{pmatrix},$$

$$\hat{G}_v = J^{-1} \begin{pmatrix} -\rho_i \beta_3 (\zeta_x \tilde{u}_i + \zeta_y \tilde{v}_i + \zeta_z \tilde{w}_i) \\ \zeta_x \tau_{xx} + \zeta_y \tau_{xy} + \zeta_z \tau_{xz} \\ \zeta_x \tau_{yx} + \zeta_y \tau_{yy} + \zeta_z \tau_{yz} \\ \zeta_x \tau_{zx} + \zeta_y \tau_{zy} + \zeta_z \tau_{zz} \\ \zeta_x \beta_x + \zeta_y \beta_y + \zeta_z \beta_z \end{pmatrix},$$

with

$$\tau_{xx} = \lambda(u_x + v_y + w_z) + 2\mu u_x,$$

$$\tau_{xy} = \tau_{yx} = \mu(u_y + v_x),$$

$$\begin{aligned}
\tau_{xz} &= \tau_{zx} = \mu(u_z + w_x), \\
\tau_{yy} &= \lambda(u_x + v_y + w_z) + 2\mu v_y, \\
\tau_{yz} &= \tau_{zy} = \mu(v_z + w_y), \\
\tau_{zz} &= \lambda(u_x + v_y + w_z) + 2\mu w_z, \\
\beta_x &= u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - q_x, \\
\beta_y &= u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - q_y, \\
\beta_z &= u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - q_z,
\end{aligned}$$

and

$$\begin{aligned}
q_x &= -\beta_2 \kappa \frac{\partial T}{\partial x} + \beta_3 \sum_{i=1}^{N_s} \rho_i h_i \tilde{u}_i, \\
q_y &= -\beta_2 \kappa \frac{\partial T}{\partial y} + \beta_3 \sum_{i=1}^{N_s} \rho_i h_i \tilde{v}_i, \\
q_z &= -\beta_2 \kappa \frac{\partial T}{\partial z} + \beta_3 \sum_{i=1}^{N_s} \rho_i h_i \tilde{w}_i,
\end{aligned}$$

where $\tilde{u}$, $\tilde{v}$, and $\tilde{w}$ are the species diffusion velocities in Cartesian coordinates. Here subscript i represents any species between 1 and N_s , where N_s is the number of species considered in the gas model. And finally the N_s component vector of chemical species production terms $\hat{H}$ is given by

$$H = J^{-1} \begin{pmatrix} \dot{W}_i \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

In addition to Eq. (1), the following global species continuity and state equations are also used:

$$\rho = \sum_{i=1}^{N_s} \rho_i, \quad (2)$$

$$p = \sum_{i=1}^{N_s} \rho_i h_i + \frac{1}{2} \rho (u^2 + v^2 + w^2) - e, \quad (3)$$

$$p = \beta_1 T \sum_{i=1}^{N_s} (\rho_i / M_i). \quad (4)$$

The diffusion velocities are found by solving the following $3N_s$ multi-component diffusion equations:

$$\xi_x \frac{\partial X_i}{\partial \xi} + \eta_x \frac{\partial X_i}{\partial \eta} + \zeta_x \frac{\partial X_i}{\partial \zeta} = \sum_{j=1}^{N_s} \frac{X_i X_j}{D_{ij}} (\tilde{u}_j - \tilde{u}_i) + (f_i - X_i) \frac{1}{p} [\xi_x p_\xi + \eta_x p_\eta + \zeta_x p_\zeta], \quad (5)$$

$$\xi_y \frac{\partial X_i}{\partial \xi} + \eta_y \frac{\partial X_i}{\partial \eta} + \zeta_y \frac{\partial X_i}{\partial \zeta} = \sum_{j=1}^{N_s} \frac{X_i X_j}{D_{ij}} (\tilde{v}_j - \tilde{v}_i) + (f_i - X_i) \frac{1}{p} [\xi_y p_\xi + \eta_y p_\eta + \zeta_y p_\zeta], \quad (6)$$

$$\xi_z \frac{\partial X_i}{\partial \xi} + \eta_z \frac{\partial X_i}{\partial \eta} + \zeta_z \frac{\partial X_i}{\partial \zeta} = \sum_{j=1}^{N_s} \frac{X_i X_j}{D_{ij}} (\tilde{w}_j - \tilde{w}_i) + (f_i - X_i) \frac{1}{p} [\xi_z p_\xi + \eta_z p_\eta + \zeta_z p_\zeta], \quad (7)$$

where f_i and X_i represent the mass fraction and the molar fraction of i -th species. In order to avoid the triviality arising from the N_s equations represented by each of the Eqs. (5), (6) and (7), any one equation from each set is to be replaced by the global conservation equations

$$\sum_{i=1}^{N_s} \rho_i \tilde{u}_i = \sum_{i=1}^{N_s} \rho_i \tilde{v}_i = \sum_{i=1}^{N_s} \rho_i \tilde{w}_i = 0. \quad (8)$$

The following non-dimensionalization has been employed in the above formulation:

$$\begin{aligned} x, y, z &= \frac{x^*, y^*, z^*}{L^*}, \quad u, v, w = \frac{u^*, v^*, w^*}{V_\infty^*}, \quad \tau = \frac{t^*}{L^*} V_\infty^*, \quad \rho = \frac{\rho^*}{\rho_\infty^*}, \\ p &= \frac{p^*}{\rho_\infty^* V_\infty^{*2}}, \quad e = \frac{e^*}{\rho_\infty^* V_\infty^{*2}}, \quad T = \frac{T^*}{T_\infty^*}, \quad h = \frac{h^*}{V_\infty^{*2}}, \\ \tilde{u}, \tilde{v}, \tilde{w} &= \frac{\tilde{u}^*, \tilde{v}^*, \tilde{w}^*}{D_\infty^*} L^*, \quad \dot{W} = \frac{\dot{W}^*}{\rho_\infty^* V_\infty^*} L^*, \quad \mu = \frac{\mu^*}{\mu_\infty^*}, \quad \kappa = \frac{\kappa^*}{\kappa_\infty^*}, \\ D &= \frac{D^*}{D_\infty^*}, \quad M = \frac{M^*}{M_\infty^*}, \quad C_p = \frac{C_p^*}{V_\infty^{*2}} T_\infty^*. \end{aligned} \quad (9)$$

Here the superscript $*$ represents dimensional variables and the subscript ∞ represents freestream values. The other constants appearing due to normalization are

$$\text{Re} = \frac{\rho_\infty^* V_\infty^* L^*}{\mu_\infty^*}, \quad \beta_1 = \frac{R_0 T_\infty^*}{M_\infty^* V_\infty^{*2}}, \quad \beta_2 = \frac{T_\infty^* \kappa_\infty^*}{\mu_\infty^* V_\infty^{*2}}, \quad \beta_3 = \frac{\rho_\infty^* D_\infty^*}{\mu_\infty^*}. \quad (10)$$

Thin Layer Approximations:

The grid system is chosen such that the body surface maps into $\eta = \text{constant}$ grid surface. While no assumptions are made on molecular diffusion terms, the thin layer approximation [13] is used for the viscous fluxes. All the diffusion terms are retained because even in our previous inviscid calculations [14] strong gradients in species concentrations were found between shock and body surfaces and therefore the molecular diffusion in our problems is no longer limited to boundary layers. Under the thin layer approximation, viscous diffusion process parallel to the body surface is neglected and no assumptions are made to the pressure. The viscous fluxes of Eq. (1) are thus simplified to

$$\hat{E}_v = J^{-1} \begin{pmatrix} -\rho_i \beta_3 (\xi_x \tilde{u}_i + \xi_y \tilde{v}_i + \xi_z \tilde{w}_i) \\ 0 \\ 0 \\ 0 \\ -\xi_x q_x - \xi_y q_y - \xi_z q_z \end{pmatrix},$$

$$\begin{pmatrix} -\rho_i \beta_3 (\eta_x \tilde{u}_i + \eta_y \tilde{v}_i + \eta_z \tilde{w}_i), \\ \mu (\eta_x^2 + \eta_y^2 + \eta_z^2) u_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_x, \\ \mu (\eta_x^2 + \eta_y^2 + \eta_z^2) v_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_y, \\ \mu (\eta_x^2 + \eta_y^2 + \eta_z^2) w_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_z \end{pmatrix}$$

$$\hat{F}_v = J^{-1} \begin{pmatrix} \mu(\eta_x^2 + \eta_y^2 + \eta_z^2)w_\eta + \frac{\mu}{3}(\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta)\eta_z, \\ \mu(\eta_x^2 + \eta_y^2 + \eta_z^2)(uu_\eta + vv_\eta + ww_\eta) \\ + \frac{\mu}{3}(\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta)(\eta_x u + \eta_y v + \eta_z w), \\ -\eta_x q_x - \eta_y q_y - \eta_z q_z, \end{pmatrix}$$

and

$$\hat{G}_v = J^{-1} \begin{pmatrix} -\rho_i \beta_3 (\zeta_x \tilde{u}_i + \zeta_y \tilde{v}_i + \zeta_z \tilde{w}_i) \\ 0 \\ 0 \\ 0 \\ -\zeta_x q_x - \zeta_y q_y - \zeta_z q_z \end{pmatrix}.$$

Here it is understood that the Cartesian derivatives are to be expanded in (ξ, η, ζ) space via chain rule relations such as

$$u_x = \xi_x u_\xi + \eta_x u_\eta + \zeta_x u_\zeta.$$

Chemical Kinetics:

In the present calculation, the gas model consists of the five species; (i) molecular oxygen O_2 , (ii) atomic oxygen O , (iii) molecular nitrogen N_2 , (iv) atomic nitrogen N and (v) nitric oxide NO . The following reactions are considered among the constituent species:

Here M is any third molecule serving to absorb excess energy released during the collision process. The forward reaction rate of j -th reaction is given by the modified Arrhenius law

$$k_{fj} = S_j T^{*\beta_j} \exp(-E_{aj}/R_0 T^*). \quad (11)$$

The values of S , β and E_a are taken from Reference 15. The backward reaction rate is obtained from the relation

$$k_{bj}=k_{ff}/K_{cj}, \quad (12)$$

where K_c is the concentration equilibrium constant, a function of temperature only. An empirical formula given by Park [15]

$$\begin{aligned} K_{cj} &= \exp (A_{j1} + A_{j2} \ln Z + A_{j3} Z + A_{j4} Z^2 + A_{j5} Z^3), \\ Z &= 10000/T^*, \end{aligned} \quad (13)$$

is used. All the constants appearing in the above equations for all the reactions considered are also listed in Ref. 15. Once the forward and backward reaction rates have been determined, the production rates of the five species can be obtained from the law of mass action. For the general chemical reaction

$$\sum_{i=1}^{N_s} \nu'_{ji} c_i \rightleftharpoons \sum_{i=1}^{N_s} \nu''_{ji} c_i, \quad j=1, \dots, N_r, \quad (14)$$

the law of mass action can be written for the rate of production of i -th species by j -th reaction as follows:

$$(\dot{W}_i^*)_j = (\nu''_{ji} - \nu'_{ji}) M_i \left[k_{ff} \prod_{i=1}^{N_s} c_i^{\nu'_{ji}} - k_{bj} \prod_{i=1}^{N_s} c_i^{\nu''_{ji}} \right]. \quad (15)$$

The net rate of production of i -th species due to all the reactions is then found by summing up the contributions from each reaction,

$$\dot{W}_i^* = \sum_{j=1}^{N_r} (\dot{W}_i^*)_j. \quad (16)$$

Thermodynamic Model:

The enthalpy and specific heat of the mixture are obtained from the following expressions:

$$h^* = \sum_{i=1}^{N_s} f_i h_i^*, \quad (17)$$

$$C_{pi}^* = \sum_{i=1}^{N_s} f_i C_{pi}^*, \quad (18)$$

where h_i^* and C_{pi}^* are the dimensional enthalpy and specific heat, respectively, of the i -th species. The values for h_i and C_{pi}^* as functions of temperature for all the species considered are obtained from the tables prepared by extending the JANAF Table [16]. Cubic spline interpolation is used to obtain values at any intermediate temperature.

Diffusion Models:

The individual species viscosity is obtained from Sutherland's law

$$\frac{\mu^*}{\mu_0} = \left(\frac{T^*}{T_0} \right)^{3/2} \left(\frac{T_0 + S}{T^* + S} \right), \quad (19)$$

where μ_0 and T_0 are the reference values and S the Sutherland constant. All the three values are taken from the tables given in Reference 17]. Once the viscosity of each species is determined, the mixture viscosity is determined from Wilke's law [18]

$$\mu^* = \sum_{i=1}^{N_s} \frac{\mu_i^*}{1 + \frac{1}{X_i} \sum_{j=1, j \neq i}^{N_s} X_j \phi_{ij}}, \quad (20)$$

where

$$\phi_{ij} = \frac{\{1 + [(\mu_i^*/\mu_j^*)(\rho_j/\rho_i)]^{1/2}(M_i/M_j)^{1/4}\}^2}{\frac{4}{2}[1 + (M_i/M_j)]^{1/2}}. \quad (21)$$

The species thermal conductivity is also given by Sutherland's law

$$\frac{k^*}{k_0} = \left(\frac{T^*}{T_0}\right)^{3/2} \left(\frac{T' + S'}{T^* + S'}\right), \quad (22)$$

The values of k_0 , T_0' and the second Sutherland constant S' are also obtained from Reference 17. Using these individual species conductivities, the mixture thermal conductivity is obtained using Wassilewas's formula [19]

$$k^* = \sum_{i=1}^{N_s} \frac{k_i^*}{1 + \frac{1}{X_i} \sum_{j=1, j \neq i}^{N_s} X_j \phi'_{ij}}, \quad (23)$$

where $\phi'_{ij} = 1.065 \phi_{ij}$ and ϕ_{ij} is given in Eq. (21).

The binary diffusion coefficient D_{ij}^* between species i and j is calculated from the empirical formula given by Chapman and Cowling [17]

$$D_{ij}^* = \frac{0.001858 T^{*3/2} [(M_i^* + M_j^*)/(M_i^* M_j^*)]^{1/2}}{p^* \sigma_{ij}^2 \Omega_D}. \quad (24)$$

Here the diffusion collision integral is approximated by

$$\Omega_D = T_*^{-0.145} + (T_* + 0.5)^{-2}, \quad (25)$$

where

$$T_* = T^*/T_{\epsilon ij}.$$

Values of the effective temperature T_ϵ and effective collision diameter σ are taken to be averages of the separate molecular properties of each species [17];

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j), \quad (26)$$

$$T_{\epsilon ij} = (T_{\epsilon i} T_{\epsilon j})^{1/2}. \quad (27)$$

Once the binary diffusion coefficients for all the species combinations are known, the diffusion velocity of each species can be computed from Eqs. (5) through (8). At any time level of computation, even though these equations form a system of simultaneous algebraic equations, some attention is required in solving them. In case any particular species is absent anywhere in the flow domain, the corresponding equation in Eq. (5) through (7) will vanish and this poses a severe problem for automatic computation. This difficulty has been resolved in the present study without sacrificing any computational efficiency by using a modified form of Gauss elimination process.

GRID SYSTEM

Flowfields around the nose portion of a reentering spacecraft are solved in the present study. The body geometry consists of a sphere-cone portion and a long cylindrical after-body. A moving body-oriented coordinate system, shown in Fig. 1, has been chosen. The grid system consists of fixed radial rays ($\xi=\text{const}$ and $\zeta=\text{const}$) and floating $\eta=\text{const}$ surfaces. The innermost $\eta=\text{const}$ surface agrees with the body surface and the outermost one always agrees with the moving shock surface. All the other $\eta=\text{const}$ grid surfaces filling the shock layer are distributed exponentially between these two boundary surfaces. Exponential stretching is used to allow grid points to concentrate near the body and peripheral shock surfaces. Clustering grid points near the shock surface is necessary to resolve the rapid change in chemical species immediately downstream of the shock wave.

NUMERICAL SCHEME

A finite-difference form of the governing equations has to be integrated between the shock and body surfaces from the given initial conditions to yield a time-evolving solution. Since we are interested only in a steady solution, the integration in time should be carried out until the solution converges to a steady-state one. Once the solution becomes steady, it is assumed that the peripheral shock has moved to its equilibrium position and all the mesh velocities at all grid points have become zero. The governing equations given by Eq. (1) are approximated by adopting the non-iterative approximately-factorized implicit method of Beam and Warming and are solved in the following three steps:

$$\begin{aligned} (I + \Delta\tau\delta_\xi\hat{A}^n - \Delta\tau \text{Re}^{-1} \delta_\xi J^{-1} \hat{P}^n J - \epsilon_\mu J^{-1} \nabla_\xi \Delta_\xi J) \Delta\tilde{q} \\ = -\Delta\tau[\delta_\xi\hat{E}^n + \delta_\eta\hat{F}^n + \delta_\zeta\hat{G}^n - \text{Re}^{-1}(\delta_\xi\hat{E}_v^n + \delta_\eta\hat{F}_v^n \\ + \delta_\zeta\hat{G}_v^n) - \hat{H}^n] - \epsilon_E J^{-1}[(\nabla_\xi \Delta_\xi)^2 + (\nabla_\eta \Delta_\eta)^2 + (\nabla_\zeta \Delta_\zeta)^2] J \hat{q}, \end{aligned} \quad (28)$$

$$(76I + \Delta\tau\delta_\eta\hat{B}^n - \Delta\tau \text{Re}^{-1} \delta_\eta J^{-1} \hat{Q}^n J - \epsilon_\mu J^{-1} \nabla_\eta \Delta_\eta J) \Delta\tilde{q} = \Delta\tilde{q}, \quad (29)$$

$$(I + \Delta\tau\delta_\zeta\hat{C}^n - \Delta\tau \text{Re}^{-1} \delta_\zeta J^{-1} \hat{R}^n J - \epsilon_\mu J^{-1} \nabla_\zeta \Delta_\zeta J) \Delta\hat{q} = \Delta\tilde{q}, \quad (30)$$

and the solution is updated using

$$\hat{q}^{n+1} = \hat{q}^n + \Delta \hat{q} . \quad (31)$$

Here the δ 's are central-difference operators, while Δ and ∇ are forward and backward-difference operators, respectively. The Jacobian matrices

$$\begin{aligned} \hat{A}^n &= \frac{\partial \hat{E}^n}{\partial \hat{q}^n}, \quad \hat{B}^n = \frac{\partial \hat{F}^n}{\partial \hat{q}^n}, \quad \hat{C}^n = \frac{\partial \hat{G}^n}{\partial \hat{q}^n}, \\ \hat{P}^n &= \frac{\partial \hat{E}_v^n}{\partial \hat{q}^n}, \quad \hat{Q}^n = \frac{\partial \hat{F}_v^n}{\partial \hat{q}^n}, \quad \hat{R}^n = \frac{\partial \hat{G}_v^n}{\partial \hat{q}^n}, \end{aligned} \quad (32)$$

represent the time linearization of the fluxes the elements of which are given in Appendix. In the linearization of viscous and diffusion fluxes, all the transport properties are assumed to be locally constant and the diffusion velocities are replaced by the concentration gradients using Fick's Law [12].

Fourth-order dissipation terms are added to the explicit portion of Eqs. (28) to (30) while second-order dissipation terms are added implicitly. The fourth-order dissipation coefficient ϵ_E is set equal to $\Delta \tau$ and ϵ_1 is made equal to $2 \epsilon_E$. The left hand side of Eqs. (28) through (30) yields a block-tridiagonal system of equations with $(N_s+4) \times (N_s+4)$ block matrices. For the five-species-gas model considered in the present formulation, the blocks are square matrices of order 9. The block-tridiagonal system is solved on vector computers efficiently by vectorizing the operations globally.

Decoding the Physical Variables:

Once all the physical variables at n -th time step are known, then by solving Eqs. (28) through (31) the conservational variables $\hat{q}$ at $(n+1)$ -th time step can be calculated. The physical variables ρ_i , u , v , w , p and T must be decoded from the conservational variables $\hat{q}$ in order to proceed to the next integration step. ρ_i , u , v and w can be obtained directly from the conservational variables ρ_i , ρu , ρv and ρw . In order to decode the pressure and temperature, a table look-up/curve-fitting procedure is adopted.

By using the state equation (4), the pressure relation (3) can be rewritten as follows:

$$T = \frac{1}{\beta_1 \sum_{i=1}^{N_s} (\rho_i / M_i)} \left[\sum_{i=1}^{N_s} \rho_i h_i + \frac{1}{2} \rho (u^2 + v^2 + w^2) - e \right] . \quad (33)$$

Since ρ_i , u , v , w and e are known, the above equation can be written as

$$T = a \sum_{i=1}^{N_s} \rho_i h_i + b . \quad (34)$$

From the physical data we know h_i^* as a piecewise cubic spline function of temperature T^* :

$$h_i^* = h_i^*(T^*) . \quad (35)$$

Eqs. (34) and (35) are solved by using Newton-Raphson method for T^* and h_i^* . Once the temperature and enthalpy are known, the pressure can be calculated from Eq. (3).

BOUNDARY CONDITIONS

Since low and moderate angles of attack are considered in the present analysis, the flow is assumed to be symmetric about a plane passing through the incoming velocity vector and the body axis, and therefore only one half of the flowfield is considered. Five kinds of boundaries, i.e. (i) body surface, (ii) shock surface, (iii) exit flow plane, (iv) plane of symmetry and (v) the singular line are encountered in this formulation. All the unknown values of $\hat{q}$ on these boundaries are updated explicitly.

(i) Body Surface: For viscous flows, ρ is extrapolated at the grid points on the body surface from the nearby grid points in the flowfield, and all the velocity components u , v and w are set equal to zero. The surface pressure is obtained from the normal momentum relation [13]

$$\frac{\partial p}{\partial n} = (\xi_x \eta_x + \xi_y \eta_y + \xi_z \eta_z) p_\xi + (\eta_x^2 + \eta_y^2 + \eta_z^2) p_\eta + (\zeta_x \eta_x + \zeta_y \eta_y + \zeta_z \eta_z) p_\zeta = 0. \quad (36)$$

The following boundary conditions are imposed for temperature and species concentrations:

(a) Adiabatic and non-catalytic wall;

$$\frac{\partial T}{\partial n} = 0 \text{ and } \frac{\partial f_i}{\partial n} = 0, \quad i=1 \text{ to } N_s.$$

(b) Isothermal and non-catalytic wall;

$$T = T_w \text{ and } \frac{\partial f_i}{\partial n} = 0, \quad i=1 \text{ to } N_s.$$

(c) Isothermal and fully-catalytic wall;

$$T = T_w \text{ and } f_i = f_{i\infty}, \quad i=1 \text{ to } N_s.$$

(ii) Shock Surface: The peripheral bow shock that separates the disturbed flow from freestream is treated as sharp discontinuity, forming a boundary. Note that the flow only in the continuum mechanics regime is considered in the present analysis. However, at very high altitudes, ionization is significant where the free electrons could diffuse upstream of the shock and can invalidate the present approach; such flows are out of scope of the present study. This shock boundary is allowed to move freely on radial rays and the movement of shock on each ray is determined by integrating

$$\frac{d}{d\tau}(\Delta\eta_s) = w_s, \quad (37)$$

where w_s is the velocity of the shock on a radial ray.

The shock velocity w_s is calculated using the shock pressure p_2 which is extrapolated from the field points, and by solving iteratively the Rankine-Hugoniot relations for the moving discontinuity simultaneously with the cubic spline curves fitted to the

thermodynamic data. The frozen shock conditions are explicitly imposed by allowing no reactions across the shock wave. The other details on the shock treatment can be found in References 14 and 20.

(iii) Exit Boundary: All the flow variables on this boundary are extrapolated from the upstream values.

(iv) Plane of Symmetry: The grid system is chosen such that a pair of windward and leeward planes ($\xi=\text{const}$) adjacent to the calculation domain lie across the plane of symmetry. Flow variables on these planes are obtained by applying the reflecting image principle, i.e. all the flow variables except w are reflected symmetrically while w is reflected anti-symmetrically such that $w=0$ on the plane of symmetry.

(v) Singular Line: Though a limiting form of the governing equations is to be used on the singular line, the choice of spherical body-oriented coordinate system allows us to avoid the singularity in the finite-difference formulation. But in order to use consistent dissipative terms in ξ -direction near the singular line, it is necessary to know the values of the conservational variables on the singular line. Simple extrapolation procedure is used in the present formulation.

STABILITY AND INITIAL CONDITIONS

If the chemical production terms $\dot{W}_i$ were identically equal to zero, then a linear stability analysis suggests [21]

$$\Delta\tau^* = \min \left\{ \frac{\Delta\xi}{\lambda_{\max}}, \frac{\Delta\eta}{\mu_{\max}}, \frac{\Delta\zeta}{\theta_{\max}} \right\}, \quad (38)$$

where $\lambda_{\max}$, $\mu_{\max}$ and $\theta_{\max}$ are the eigenvalues of the matrices $\hat{A}^n$, $\hat{B}^n$ and $\hat{C}^n$, respectively. Although the production term $\dot{W}_i$ is too complex for a stability criterion on $\Delta\tau$ to be determined analytically, an empirical condition can be derived from the consideration of chemical relaxation times. In the present study, it is found that the relation $\Delta\tau=0.2\Delta\tau^*$ allows a stable integration process. As a CFL value equal to 10 works out well for non-reacting real gases, a CFL number equal to 2 is used throughout reacting flow calculations. The initial data for reacting flow calculations are supplied from the non-reacting real gas code.

RESULTS AND DISCUSSIONS

Calculations are made for non-equilibrium flows on the grid system shown in Fig. 1 at various Mach numbers. The simplified body configuration is obtained by smoothly joining a sphere head of radius R and a conical cylinder of 20° half angle. An air mixture of 21 percent oxygen and 79 percent nitrogen at an altitude 70 km is chosen as freestream. The ambient pressure and temperature are 5.5 kg/m^2 and 218.36 K , respectively. The chosen Mach numbers 15, 20 and 25 correspond to the flight velocities 4.45, 5.94 and 7.42 km/s , respectively. The other freestream conditions are as follows:

Fig. 1. The coordinate system, the body geometry and the grid system.

$$\gamma_f=1.3972, \quad Pr=1.1171, \quad Le=1.0101, \quad Sc=1.1284,$$

and

$$Re=2.994 \times 10^4 \quad (\text{at } M_f=25).$$

Based on the gas model and the chosen boundary conditions, all the numerical results presented here are categorized into the following five cases:

- Case I: A real gas (non-reacting) model with adiabatic wall.
- Case II: A real gas (non-reacting) model with isothermal wall ($T_w=1200\text{K}$).
- Case III: A chemically reacting gas model with adiabatic wall.
- Case IV: A chemically reacting gas model with isothermal ($T_w=1200\text{K}$) and non-catalytic wall.
- Case V: A chemically reacting gas model with isothermal ($T_w=1200\text{K}$) and fully-catalytic wall.

The grid system consists of 46 points in ξ -direction, 40 points in η -direction between body and peripheral bow shock and 20 points in ζ -direction. Clustering of grid points in η -direction near the shock and body is changed during the solution process based on the intermediate solutions. After carefully vectorizing the codes, all calculations are performed on FUJITSU's either VP-200 or VP-400 vector computer at National Aerospace Laboratory. Although the present analysis requires inversion of 9×9 block matrices and frequent data searching, which can only be partially vectorized, these

codes took only 4.52×10^{-4} seconds per grid point per step for the three-dimensional flow and 2.28×10^{-4} seconds per grid per step for the two-dimensional flow. After starting from the non-reacting real gas solutions, about 5000 time steps are required to obtain a converged solution for a chemically reacting flow.

Results for Two-Dimensional Flows:

In order to explore in detail the non-equilibrium phenomena associated with the present flow conditions, a number of calculations are performed initially on a two-dimensional plane body. Shock standoff distances obtained for the three Mach numbers considered are tabulated in Table 1 and the shock shapes for Mach number 25 are shown in Fig. 2. All the inviscid solutions are taken from Reference 14. If the chemically reacting viscous gas model with isothermal wall conditions is assumed to represent the actual flow conditions most accurately, then Table 1 tells us how far the results obtained with other gas models are from the actual values. The real gas models which are calorically imperfect but chemically inert are bringing shocks close to the

Table 1. Shock Standoff Distances for a Two-Dimensional Blunt Body in Perfect Gas, Real Gas, and Chemically Reacting Gas Models.

Mach Number	Flight Speed*	Shock Standoff Distance δ/R						
		Perfect Gas	Real Gas			Chemically Reacting Gas		
			Inviscid	Viscous		Inviscid	Viscous	
				Adiabatic Wall	Isothermal Wall		Adiabatic N. C. Wall	Isothermal N. C. Wall Isothermal F. C. Wall
15	4.45	0.40294	0.29910	0.30006	0.29991	0.20494	0.23729	0.22744 0.23571
20	5.93	0.38311	0.28289	0.28361	0.28330	0.14768	0.17197	0.16305 0.16714
25	7.42	0.37196	0.27029	0.27108	0.26998	0.10952	0.13494	0.13562 0.13939

* Flight Speed in km/S.

Fig. 2. Shock shapes for an adiabatic wall at Mach number 25.

body but are still not sufficient to describe hypersonic flow accurately. Chemically reacting inviscid gas model is predicting the shocks closest to the body. Boundary layers are effectively changing the body shape and in turn pushing the shocks away (Fig. 2). The molecular diffusion considered in the chemically reacting viscous models is further pushing away the bow shocks. A lower temperature of an isothermal wall is thinning the boundary layer due to the lower viscosity and hence is relaxing the shock wave. It should be noted that all these results are for a two-dimensional plane body; the effects are not so severe for an axis-symmetric or three-dimensional body.

The surface pressure coefficient is defined as

$$c_p = \frac{p_w^* - p_\infty^*}{\frac{1}{2} \rho_\infty^* V_\infty^{*2}}, \quad (39)$$

the variation of which along the body for real gas and reacting gas models is compared in Fig. 3. Near the stagnation point chemical reactions are not affecting the surface pressure but in the downstream higher surface pressure coefficients are predicted by the reacting gas model.

The skin friction coefficient obtained from the equation

$$c_f = \frac{\tau_w^*}{\frac{1}{2} \rho_\infty^* V_\infty^{*2}}, \quad (40)$$

where

$$\tau_w^* = \mu_w^* \left. \frac{\partial V^*}{\partial n} \right|_w,$$

is plotted in Figs. 4 and 5 for all the five cases considered for the Mach numbers 15 and 25, respectively. A lower wall temperature of an isothermal wall ($T_w = 1200\text{K}$) reduces the viscosity and the resulting velocity gradient near the wall is large due to the

Fig. 3. Wall pressure coefficient obtained with real and chemically reacting gas models.

thinning of the boundary layer. Since the skin-friction coefficient is a strong function of temperature for high Reynolds number flows, isothermal walls give less skin friction than adiabatic walls. Chemical reactions drop the temperature further and consequently the skin friction. Surprisingly, a fully-catalytic wall increases the skin friction, as seen in Figs. 4 and 5. This increase is due to the increased concentrations of nitrogen and oxygen molecules near the body which have larger viscosity coefficients

Fig. 4. Comparison of wall skin-friction coefficient at Mach number 15.

Fig. 5. Comparison of wall skin-friction coefficient at Mach number 25.

than atoms.

Stanton number is defined as

$$St = \frac{-q_w^*}{\rho_\infty^* V_\infty^* (H_\infty^* - H_w^*)}, \quad (41)$$

where H^* is the total enthalpy given by

$$H = h + \frac{1}{2}(u^2 + v^2 + w^2), \quad (42)$$

and the total heat transfer (from body to fluid) q_w^* is calculated from

$$q_w^* = -k_w^* \frac{\partial T^*}{\partial n} \Big|_{wall} + \sum_{i=1}^{N_s} \rho_i^* h_i^* \tilde{v}_i^*, \quad (43)$$

Fig. 6. Wall Stanton number compared for different cases at $M=15$.

Fig. 7. Wall Stanton number compared for different cases at $M=25$.

where $\bar{v}_i^*$ is the non-dimensional diffusion velocity of i -th species normal to the body. The first term in Eq. (43) is the conductive heating rate while the second the diffusive heating rate. Stanton number for the two Mach numbers are shown in Figs. 6 and 7. Note that conductive heat transfer to an adiabatic wall and diffusive heat transfer to a non-catalytic wall are identically zero. At Mach number 25 Stanton number is substantially increased for a fully-catalytic wall, indicating increased heating of the wall by the flow. The diffusive heat transfer Q_D (kilowatts/m²) is plotted for the three Mach numbers in Fig. 8. Negative Q_D indicates that heat is transferred from flow to body. Interestingly, the reversal of heat transfer from flow to body is taking place for all the March numbers at the same location on the body, $\xi=0.9961$ corresponding to a point of intersection of the 57.07° radial line and the sphere head.

Fig. 8. Wall heat transfer due to molecular diffusion.

Fig. 9. Velocity vectors in a chemically reacting flow at $M=15$.

Velocity vectors in a chemically reacting flow at Mach number 15 are shown in Fig. 9, where growth of boundary layer can easily be identified. In Fig. 10 constant-temperature contours are shown for various cases at Mach number 25. A thick thermal boundary layer for the non-reacting flow (Fig. 10 (a)) and a relatively thin thermal boundary layer for reacting flows can be identified. In addition in a reacting flow, a well defined thermal boundary layer exists near the shock wave where severe chemical reactions are taking place. Such a layer can be realized accurately only by using a sharp shock method. A smeared shock that is captured by a shock capturing technique diffuses into this reacting layer giving only the equilibrium values.

Temperature and mass fraction distributions along stagnation streamline ($\xi=0$) are shown in Figs. 11 through 14. The distance indicated on x -axis is the normalized one between body and shock. Freestream air starts dissociating immediately after passing through the bow shock and the temperature drops rapidly. At these high temperatures, oxygen molecule has completely dissociated near the shock and thereafter only a trace of O_2 can be found. Nitric oxide is formed at the shock wave and then rapidly dissociates. Within the wall boundary layer atomic nitrogen recombines into N_2 . This recombination decreases the density near the wall and hence even though there is no molecule to produce oxygen atom, the mass fraction of oxygen atom increases (Figs. 12, 13). A fully-catalytic wall (Fig. 14) requests all the species mass fractions equal to

Fig. 10. Constant-temperature contours.

Fig. 11. Temperature Variation between Body and Shock along the Stagnation Streamline.

Fig. 12. Mass Fraction Profiles along Stagnation Streamline for Case III.

the corresponding freestream values. This leads to a spike-like reappearance of oxygen molecules near the wall.

Similar plots at a far downstream location, $\xi = 3.234$, are shown in Figs. 15 through 18. From temperature graphs it is noticed that the initial drop in temperature near the shock is due to the dissociation of molecular nitrogen and oxygen and then temperature increases due to the adiabatic compression. Even at this location, oxygen molecules are completely dissociated. Reformation of oxygen molecules near the body with fully-catalytic wall (Fig. 18) results into a diffused oxygen atom profile unlike a spike developed near the stagnation point; on the other hand a spike in the nitric oxide density is formed within the boundary layer.

Fig. 13. Mass Fraction Profiles along Stagnation Streamline for Case IV.

Fig. 14. Mass Fraction Profiles along Stagnation Streamline for Case V.

All the results obtained at different Mach numbers and boundary conditions over a two-dimensional body are consistent and agree with the physics of the fluid. For each case a VP-200 computer took about 30 minutes cpu time. Extension of these calculations to a three-dimensional flow increased the computer time to 3 to 4 hrs. *Results for a Three-Dimensional Flow:*

Calculations are performed on an axi-symmetric body shown in Fig. 1 at Mach number 20 and angle of attack $\alpha=7.5^\circ$. Solution at this angle of attack is developed step by step starting from zero angle of attack solution. Pressure coefficients c_p on an isothermal non-catalytic wall in the plane of symmetry ($\zeta=0^\circ$ and 180°) are calculated using Eq. (39) and are shown in Fig. 19. Flow at this angle of attack is truly laminar

Fig. 15. Temperature Variation between Body and Shock along the Radial Line $\xi=3.234$.

Fig. 16. Mass Fraction Profiles along Radial Line $\xi=3.234$ for Case III.

and no crossflow separation is noticed. Due to the angle of attack, the pressure coefficient is marginally increased on the windward side ($\zeta=0^\circ$) whereas it is appreciably decreased on the leeward side ($\zeta=180^\circ$). Variation of wall Stanton number is shown in Fig. 20. As the wall is non-catalytic, the contribution due to molecular diffusion is absent. In Figs. 21 and 22 the wall skin-friction coefficients in the windward and leeward sides in the plane of symmetry are plotted. The wall skin friction is reduced from windward side to leeward side for an adiabatic wall but remains more or less the same for an isothermal wall. Fig. 23 gives constant-temperature contours in a reacting flow in the plane of symmetry. The thermal boundary layer associated with the shock is very thin at this Mach number. The

Fig. 17. Mass Fraction Profiles along Radial Line $\xi=3.234$ for Case IV.

Fig. 18. Mass Fraction Profiles along Radial Line $\xi=3.234$ for Case V.

temperature along the radial lines far downstream of the stagnation point ($\xi=3.14$) is compared for adiabatic and isothermal walls in Fig. 24, while the respective mass fraction distributions are shown in Fig. 25. Oxygen and nitrogen molecules are gradually dissociating and nitric oxide is significant near the wall. A lower temperature on the leeward side moves the point of reaction initiation further from the shock. As seen in Fig. 25 (c), only a trace of nitric oxide is formed in the entire section, even though the wall temperature is as high as the one on the windward side. This is a typical feature of finite-rate chemistry which uses different characteristic times for different reactions. The production of a particular species not only depends on the local temperature but also on the characteristic time of that reaction.

Fig. 19. Wall Pressure Coefficient in Plane of Symmetry;
 $M_t=20$, $\alpha=7.5^\circ$.

Fig. 20. Wall Stanton Number in Plane of Symmetry;
 $M_t=20$, $\alpha=7.5^\circ$.

CONCLUSIONS

A hybrid scheme that treats the peripheral shock as sharp one is successfully developed for a chemically reacting flow. Use of the non-iterative, approximately-factored implicit scheme eliminated the problem of stiffness that is present in the governing equations. Time-dependent N-S equations are solved over the entire subsonic and supersonic flow regimes simultaneously. The five species considered here are treated as calorically imperfect but thermally perfect gases. Viscous terms are simplified using the thin layer approximation whereas all the molecular diffusion transport terms are retained. Complete diffusion equations are sloved at every grid

Fig. 21. Wall Skin-Friction Coefficient in Leeward Side.

Fig. 22. Wall Skin-Friction Coefficient in Windward Side.

point and at every time step. Calculations are made for various cases and the results are validated on physical grounds. A rigorous comparison of the results with experiments is not made because of the scarcity of the relevant data. As the interest in finite-rate chemically reacting flows is increasing sharply, use of standard data for transport properties, species enthalpies and reaction rates is needed for comparison with the results obtained by other researchers using different techniques. Present

Fig. 23. Constant Temperature Lines in a Reacting Flowfield at $M_f=20$, $\alpha=7.5^\circ$.

calculations indicate that the temperature and molecular mass fractions are rapidly decreasing near the shock wave at Mach number 25, resulting in a thermal boundary layer near the shock wave. Shock fitting methods such as the one presented here have better ability to resolve these thermal layers than the shock capturing methods which capture the strong bow shock. Advantages of the shock capturing method to capture relatively weak shocks is preserved by using a hybrid formulation. Techniques for treating species production terms implicitly using two parallel codes, one for the complete equations and another for the simplified equations for the species change, are under study.

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Fig. 24. Temperature Variation in Plane of Symmetry;
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Fig. 25. Mass Fraction Profiles in Plane of Symmetry;
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APPENDIX

Inviscid Jacobian Matrices:

The inviscid Jacobian matrices $\hat{A}^n$, $\hat{B}^n$ and $\hat{C}^n$ are obtained in the time linearization of $\hat{E}^n$, $\hat{F}^n$ and $\hat{G}^n$ and the expressions for the elements of these $(N_s+4) \times (N_s+4)$ matrices are given here. If we define the quantities

$$\theta = K_1 u + K_2 v + K_3 w,$$

$$\bar{R} = \frac{\beta_1}{\rho} \sum_{i=1}^{N_s} \frac{\rho_i}{M_i},$$

$$v = (1 - C_p / \bar{R}),$$

and

$$\phi_j = [C_{pj}(T - T_f^0) + h_{fj}^0 - \frac{C_p T}{\bar{R} M_j / \beta_1} - 0.5(u^2 + v^2 + w^2)] / v,$$

where T_f^0 ($=298.0/T^*$) is the reference temperature for enthalpies and h_{fj}^0 is the heat of formation of j -th species, then the elements of inviscid Jacobian matrices can be written as follows:

$$\begin{aligned} \psi_{i,j} &= K_0 + (1 - \frac{\rho_i}{\rho})\theta & \text{if } i=j \\ &= -\frac{\rho_i}{\rho}\theta & \text{if } i \neq j \end{aligned} \quad \left. \vphantom{\psi_{i,j}} \right\}, \quad i=1, N_s; j=1, N_s.$$

$$\begin{aligned} \psi_{N_s+1,j} &= -u\theta + K_1\phi_j, & j=1, N_s. & \quad \psi_{i,N_s+1} = K_1 \frac{\rho_i}{\rho}, & i=1, N_s. \\ \psi_{N_s+2,j} &= -v\theta + K_2\phi_j, & j=1, N_s. & \quad \psi_{N_s+1,N_s+1} = K_0 + \theta + uK_1(1+1/v). \\ \psi_{N_s+3,j} &= -w\theta + K_3\phi_j, & j=1, N_s. & \quad \psi_{N_s+2,N_s+1} = vK_1 + uK_2/v. \\ \psi_{N_s+4,j} &= -(e+p)\frac{\theta}{\rho} + \theta\phi_j, & j=1, N_s. & \quad \psi_{N_s+3,N_s+1} = wK_1 + uK_3/v. \\ \psi_{i,N_s+2} &= K_2 \frac{\rho_i}{\rho}, & i=1, N_s. & \quad \psi_{N_s+4,N_s+1} = (e+p)\frac{K_1}{\rho} + u\theta/v. \\ \psi_{N_s+1,N_s+2} &= uK_2 + vK_1/v & & \quad \psi_{i,N_s+3} = K_3 \frac{\rho_i}{\rho}, & i=1, N_s. \\ \psi_{N_s+2,N_s+2} &= K_0 + \theta + vK_2(1+1/v). & & \quad \psi_{N_s+1,N_s+3} = uK_3 + wK_1/v. \\ \psi_{N_s+3,N_s+2} &= wK_2 + vK_3/v. & & \quad \psi_{N_s+2,N_s+3} = uK_3 + wK_2/v. \\ \psi_{N_s+4,N_s+2} &= (e+p)\frac{K_2}{\rho} + v\theta/v. & & \quad \psi_{N_s+3,N_s+3} = K_0 + \theta + wK_3(1+1/v). \\ \psi_{i,N_s+4} &= 0, & i=1, N_s. & \quad \psi_{N_s+4,N_s+3} = (e+p)\frac{K_3}{\rho} + w\theta/v. \\ \psi_{N_s+1,N_s+4} &= -K_1/v. & & \quad \psi_{N_s+2,N_s+4} = -K_2/v. \\ \psi_{N_s+3,N_s+4} &= -K_3/v. & & \quad \psi_{N_s+4,N_s+4} = K_0 + \theta(1-1/v). \end{aligned}$$

From the above expressions for elements,

$\hat{A}^n$ can be obtained by setting $K_0 = \xi_t$, $K_1 = \xi_x$, $K_2 = \xi_y$, $K_3 = \xi_z$ and $\psi = \hat{A}^n$,
 $\hat{B}^n$ can be obtained by setting $K_0 = \eta_t$, $K_1 = \eta_x$, $K_2 = \eta_y$, $K_3 = \eta_z$ and $\psi = \hat{B}^n$,
and $\hat{C}^n$ can be obtained by setting $K_0 = \zeta_t$, $K_1 = \zeta_x$, $K_2 = \zeta_y$, $K_3 = \zeta_z$ and $\psi = \hat{C}^n$.

Viscous Jacobian Matrices:

The diffusion velocities $\tilde{u}$, $\tilde{v}$ and $\tilde{w}$ are strong functions of species concentrations and, therefore, assuming these velocities locally constant while deriving Jacobian matrices of viscous fluxes of Eq. (1) leads to errors. A complete treatment of the diffusion velocities complicates the analysis and hence the diffusion velocities are linearized using Fick's law¹². Since these linearizations are introduced only in deriving Jacobian matrices, they would not impair the accuracy and convergence rate of the numerical algorithm, Eqs. (28) through (31).

By using Fick's law for self diffusion, $\tilde{u}$, $\tilde{v}$ and $\tilde{w}$ can be written as

$$\tilde{u}_i = -\frac{D_{ii}}{f_i} \frac{\partial f_i}{\partial x}, \quad \tilde{v}_i = -\frac{D_{ii}}{f_i} \frac{\partial f_i}{\partial y} \quad \text{and} \quad \tilde{w}_i = -\frac{D_{ii}}{f_i} \frac{\partial f_i}{\partial z}.$$

After introducing the notation

$$\begin{aligned} \tilde{\partial}_\xi &= (\xi_x^2 + \xi_y^2 + \xi_z^2) \frac{\partial}{\partial \xi} + (\xi_x \eta_x + \xi_y \eta_y + \xi_z \eta_z) \frac{\partial}{\partial \eta} + (\xi_x \varsigma_x + \xi_y \varsigma_y + \xi_z \varsigma_z) \frac{\partial}{\partial \varsigma}, \\ \tilde{\partial}_\eta &= (\eta_x \xi_x + \eta_y \xi_y + \eta_z \xi_z) \frac{\partial}{\partial \xi} + (\eta_x^2 + \eta_y^2 + \eta_z^2) \frac{\partial}{\partial \eta} + (\eta_x \varsigma_x + \eta_y \varsigma_y + \eta_z \varsigma_z) \frac{\partial}{\partial \varsigma}, \\ \tilde{\partial}_\varsigma &= (\varsigma_x \xi_x + \varsigma_y \xi_y + \varsigma_z \xi_z) \frac{\partial}{\partial \xi} + (\varsigma_x \eta_x + \varsigma_y \eta_y + \varsigma_z \eta_z) \frac{\partial}{\partial \eta} + (\varsigma_x^2 + \varsigma_y^2 + \varsigma_z^2) \frac{\partial}{\partial \varsigma}, \end{aligned}$$

the viscous fluxes of Eq. (1) are rewritten as follows:

$$\begin{aligned} \hat{E}_v &= J^{-1} \begin{pmatrix} \rho \beta_3 D_{ii} \tilde{\partial}_\xi (\rho_i/p) \\ 0 \\ 0 \\ 0 \\ \beta_2 \kappa \tilde{\partial}_\xi (T) + \rho \beta_3 \sum_{j=1}^{N_s} h_j D_{jj} \tilde{\partial}_\xi (\rho_j/\rho) \end{pmatrix}, \\ \hat{G}_v &= J^{-1} \begin{pmatrix} \rho \beta_3 D_{ii} \tilde{\partial}_\varsigma (\rho_i/p) \\ 0 \\ 0 \\ 0 \\ \beta_2 \kappa \tilde{\partial}_\varsigma (T) + \rho \beta_3 \sum_{j=1}^{N_s} h_j D_{jj} \tilde{\partial}_\varsigma (\rho_j/\rho) \end{pmatrix}, \end{aligned}$$

and

$$\begin{aligned} \hat{F}_v &= J^{-1} \begin{pmatrix} \rho \beta_3 D_{ii} \tilde{\partial}_\eta (\rho_i/\rho) \\ \mu(\eta_x^2 + \eta_y^2 + \eta_z^2) u_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_x \\ \mu(\eta_x^2 + \eta_y^2 + \eta_z^2) v_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_y \\ \mu(\eta_x^2 + \eta_y^2 + \eta_z^2) w_\eta + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \eta_z \\ \mu(\eta_x^2 + \eta_y^2 + \eta_z^2) (u u_\eta + v v_\eta + w w_\eta) + \frac{\mu}{3} (\eta_x u_\eta + \eta_y v_\eta + \eta_z w_\eta) \\ \times (\eta_x u + \eta_y v + \eta_z w) + \beta_2 \kappa \tilde{\partial}_\eta (T) + \rho \beta_3 \sum_{h=1}^{N_s} j_h D_{hh} \tilde{\partial}_\eta (\rho_h/\rho) \end{pmatrix}. \end{aligned}$$

If we define the quantities

$$\begin{aligned} l_1 &= \mu \left(\frac{4}{3} \eta_x^2 + \eta_y^2 + \eta_z^2 \right), \\ l_2 &= \mu \left(\eta_x^2 + \frac{4}{3} \eta_y^2 + \eta_z^2 \right), \\ l_3 &= \mu \left(\eta_x^2 + \eta_y^2 + \frac{4}{3} \eta_z^2 \right), \\ l_4 &= \frac{\mu}{3} \eta_x \eta_y, \quad l_5 = \frac{\mu}{3} \eta_y \eta_z, \quad l_6 = \frac{\mu}{3} \eta_x \eta_z, \end{aligned}$$

and

$$\psi = \sum_{j=1}^{N_s} D_{jj} c_{pj} \tilde{\partial}_\eta (\rho_j / \rho),$$

the expressions for the elements of the $(N_s+4) \times (N_s+4)$ viscous Jacobian matrices $\hat{P}^n$, $\hat{Q}^n$ and $\hat{R}^n$ are obtained in the time linearization of $\hat{E}^n$, $\hat{F}^n$ and $\hat{G}^n$, respectively, as shown in the following:

$$\begin{aligned} \Phi_{i,j} &= (\rho - \rho_i) \beta_3 D_{ii} \tilde{\partial}_s \left(\frac{1}{\rho} \right) \quad \text{if } j=i \\ &= -\rho_i \beta_3 D_{ii} \tilde{\partial}_s \left(\frac{1}{\rho} \right) \quad \text{if } j \neq i \end{aligned} \quad \left. \vphantom{\Phi_{i,j}} \right\}, \quad i=1, N_s; \quad j=1, N_s. \\ \Phi_{N_s+1,j} &= \pi \left\{ l_1 \frac{\partial}{\partial \eta} \left(-\frac{u}{\rho} \right) + l_4 \frac{\partial}{\partial \eta} \left(-\frac{v}{\rho} \right) + l_6 \frac{\partial}{\partial \eta} \left(-\frac{w}{\rho} \right) \right\}, \quad j=1, N_s. \\ \Phi_{N_s+2,j} &= \pi \left\{ l_4 \frac{\partial}{\partial \eta} \left(-\frac{u}{\rho} \right) + l_2 \frac{\partial}{\partial \eta} \left(-\frac{v}{\rho} \right) + l_5 \frac{\partial}{\partial \eta} \left(-\frac{w}{\rho} \right) \right\}, \quad j=1, N_s. \\ \Phi_{N_s+3,j} &= \pi \left\{ l_6 \frac{\partial}{\partial \eta} \left(-\frac{u}{\rho} \right) + l_5 \frac{\partial}{\partial \eta} \left(-\frac{v}{\rho} \right) + l_3 \frac{\partial}{\partial \eta} \left(-\frac{w}{\rho} \right) \right\}, \quad j=1, N_s. \\ \Phi_{N_s+4,j} &= \pi \left\{ l_1 \frac{\partial}{\partial \eta} \left(-\frac{u^2}{\rho} \right) + l_2 \frac{\partial}{\partial \eta} \left(-\frac{v^2}{\rho} \right) + l_3 \frac{\partial}{\partial \eta} \left(-\frac{w^2}{\rho} \right) \right. \\ &\quad \left. + l_4 \frac{\partial}{\partial \eta} \left(-\frac{2uv}{\rho} \right) + l_5 \frac{\partial}{\partial \eta} \left(-\frac{2vw}{\rho} \right) + l_6 \frac{\partial}{\partial \eta} \left(-\frac{2wu}{\rho} \right) \right\} \\ &\quad + \beta_2 \kappa \tilde{\partial}_s \left(\frac{\partial T}{\partial \rho_j} \right) + \beta_3 \left(D_{jj} \rho h_j - \sum_{i=1}^{N_s} D_{ji} \rho_i h_i \right) \tilde{\partial}_s \left(\frac{1}{\rho} \right) + \beta_3 \rho \frac{\partial T}{\partial \rho_j} \psi, \quad j=1, N_s. \\ \Phi_{i,N_s+1} &= 0, \quad i=1, N_s. \\ \Phi_{N_s+1,N_s+1} &= \pi \left\{ l_1 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \quad \Phi_{N_s+2,N_s+1} = \pi \left\{ l_4 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \\ \Phi_{N_s+3,N_s+1} &= \pi \left\{ l_6 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \\ \Phi_{N_s+4,N_s+1} &= \pi \left\{ l_1 \frac{\partial}{\partial \eta} \left(\frac{u}{\rho} \right) + l_4 \frac{\partial}{\partial \eta} \left(\frac{v}{\rho} \right) + l_6 \frac{\partial}{\partial \eta} \left(\frac{w}{\rho} \right) \right\} \\ &\quad + \beta_2 \kappa \tilde{\partial}_s \left(\frac{u}{\rho(\bar{R} - c_p)} \right) + \beta_3 \frac{u}{(\bar{R} - c_p)} \psi. \\ \Phi_{i,N_s+2} &= 0, \quad i=1, N_s. \\ \Phi_{N_s+1,N_s+2} &= \pi \left\{ l_4 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \quad \Phi_{N_s+2,N_s+2} = \pi \left\{ l_2 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \\ \Phi_{N_s+3,N_s+2} &= \pi \left\{ l_5 \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \right\}. \end{aligned}$$

$$\begin{aligned}\Phi_{N_s+4, N_s+2} = & \pi \{ l_4 \frac{\partial}{\partial \eta} (\frac{u}{\rho}) + l_2 \frac{\partial}{\partial \eta} (\frac{v}{\rho}) + l_5 \frac{\partial}{\partial \eta} (\frac{w}{\rho}) \} \\ & + \beta_2 \kappa \tilde{\partial}_s (\frac{v}{\rho(\bar{R}-\zeta_p)}) + \beta_3 (\frac{v}{(\bar{R}-\zeta_p)}) \psi .\end{aligned}$$

$$\Phi_{i, N_s+3} = 0, \quad i=1, N_a .$$

$$\Phi_{N_s+1, N_s+3} = \pi \{ l_6 \frac{\partial}{\partial \eta} (\frac{1}{\rho}) \} . \quad \Phi_{N_s+2, N_s+3} = \pi \{ l_5 \frac{\partial}{\partial \eta} (\frac{1}{\rho}) \} .$$

$$\Phi_{N_s+3, N_s+3} = \pi \{ l_3 \frac{\partial}{\partial \eta} (\frac{1}{\rho}) \} .$$

$$\begin{aligned}\Phi_{N_s+4, N_s+3} = & \pi \{ l_6 \frac{\partial}{\partial \eta} (\frac{u}{\rho}) + l_5 \frac{\partial}{\partial \eta} (\frac{v}{\rho}) + l_3 \frac{\partial}{\partial \eta} (\frac{w}{\rho}) \} \\ & + \beta_2 \kappa \tilde{\partial}_s [\frac{w}{\rho(\bar{R}-\zeta_p)}] + \beta_3 [\frac{v}{(\bar{R}-\zeta_p)}] \psi .\end{aligned}$$

$$\Phi_{i, N_s+4} = 0, \quad i=1, N_s .$$

$$\Phi_{N_s+1, N_s+4} = \Phi_{N_s+2, N_s+4} = \Phi_{N_s+3, N_s+4} = 0 .$$

$$\Phi_{N_s+4, N_s+4} = \beta_2 \kappa \tilde{\partial}_s [\frac{1}{\rho(\bar{R}-\zeta_p)}] + \beta_3 [\frac{-1}{(\bar{R}-\zeta_p)}] \psi .$$

where

$$\frac{\partial T}{\partial \rho_j} = \frac{1}{\rho(\bar{R}-\zeta_p)} [c_{pj}(T_f^0) - \frac{\beta_1 T}{M_j} - 0.5(u^2 + v^2 + w^2)]$$

In the above expressions;

to obtain $\hat{P}^n$, set $\pi=0$ and $\Phi=P^n$, and replace the operator $\tilde{\partial}_s$ with $\tilde{\partial}_\xi$,
to obtain $\hat{Q}^n$, set $\pi=1$ and $\Phi=Q^n$, and replace the operator $\tilde{\partial}_s$ with $\tilde{\partial}_\eta$,
and to obtain $\hat{R}^n$, set $\pi=0$ and $\Phi=R^n$, and replace the operator $\tilde{\partial}_s$ with $\tilde{\partial}_\zeta$.