

COMPUTATION OF UNSTEADY NONEQUILIBRIUM PROPULSIVE FLOWFIELDS

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ABSTRACT

This paper describes a scheme to numerically predict hypersonic flow fields with emphasis on temporal and nonequilibrium effects in two dimensions. The gas model allows for chemical and thermal nonequilibrium. Finite rate chemistry is used to simulate several possible reactions among 11 chemical species present in air. A two temperature model is employed to simulate the thermal nonequilibrium effects, a vibrational - electronic temperature and a rotational-translational temperature being the two temperatures used. The intended applications of this code include the simulation of partially ionized high temperature flow fields including magnetohydrodynamic (MHD) effects. To that end, the formulation includes provisions for MHD terms, which are treated as source terms in the flow equations.

INTRODUCTION

The numerical prediction of a hypersonic or high temperature flow field must account for various physical phenomena to be realistic. The most important of these effects are: (a) Chemical reactions that occur spontaneously, (b) Energy transfer among the translational, rotational, vibrational and electronic modes, (c) changes in transport properties at high temperatures and pressures, (d) surface catalysis, and (d) radiative energy transfer. While all of these effects can be quantified from physical laws, they require experimentally obtained coefficients to complete the system of equations. The quantities that must be obtained from tables, typically, are the chemical reaction rate data, curve fits for thermodynamic properties such as C_p and collision integrals that are used to determine the transport properties.

All the effects mentioned above may be included in a comprehensive system of conservation laws (ref. Gnoffo et al. [1], Park[2]). Early attempts to solve these equations centered around finding convenient similarity parameters (Dorance [3]) and using integral methods (Chung and Anderson

[4]) or finite differences (Blottner [5]) to compute them. The emphasis of these methods was upon the behaviour of hypersonic reacting boundary layers and relatively less importance was attached to the thermal nonequilibrium. An actual set of data for the system of reacting Nitrogen-Oxygen air model may be found in Ref.[1]. This is the air model that is used for the current study.

At the temperature ranges that are of interest in high temperature flows, the flow properties are affected considerably by thermal nonequilibrium by which is meant the storage of energy in several distinct modes. An elaborate treatment of the physics of nonequilibrium may be found in the works of Vincenti and Kruger [6] and Mitchener and Kruger [7] and Anderson [8]. An added feature at high temperatures is that transport properties (viscosity, thermal conductivity and diffusion coefficients) depend on intermolecular collisional rates, and can be thereby deduced from the collision integrals by methods detailed in the above references.

The current interest in introducing Magnetohydrodynamic terms in the governing equations is two-fold. (1) MHD may be used as an auxiliary propulsive device in a dual mode propulsion system, (Hill and Peterson [9]) and (2) it has been of contemporary interest to investigate the effectiveness of MHD augmented ionized nonequilibrium flow to boost the test ranges of a ground based hypersonic facility (Simmons et al. [10] and Adamovich and Rich [11]). While a flow field may be accelerated by means of MHD by seeding with an easily ionizable species, the possibility of obtaining MHD acceleration based on the increased levels of nonequilibrium ionization in an unseeded flow is very intriguing. The increase in ionization causes an increase in conductivity thereby causing a greater acceleration by means of MHD. Venable et al. [12] have recently modeled quasi one-dimensional unsteady equilibrium flow with MHD terms using upwind schemes.

This paper describes the proposed use of a two dimensional flow solver to simulate such flows with references to possible alternative methods. The flow contains several distinct time-scales: (a) The chemical reaction time scale, (b) Thermal equilibration time scale, and (c) The flow time scale. This makes the flow equations inherently stiff. This demands the use of an implicit numerical scheme to solve the flow equations, and explicit schemes will face very stringent upper bounds on the allowable time step.

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Upwind based algorithms for solving flows in thermochemical nonequilibrium have been investigated by several authors recently. The papers by Cinella and Grossman [13] and Liu and Vinokur [14] describe the upwinding strategy applied to such flows. The work by Candler and MacCormack [15] possibly represents the first successful application of a comprehensive investigation of nonequilibrium flow fields of interest. Their work includes a multi-temperature model corresponding to the individual species vibrational temperatures, the electronic temperature and a translational temperature. The numerical method used is a flux-vector split implicit scheme, which is iterated until convergence. A noniterative Parabolized Navier-Stokes based technique has been developed by Miller et al. [16]. The current method is based upon an upwind relaxation scheme developed by Gnoffo ([17] for perfect gas, and [18] for nonequilibrium air).

FLUID EQUATIONS

This section details the governing equations of a gas using a two-temperature model for thermal non-equilibrium. The two temperatures are:

(1) Heavy particle Vibrational - Electronic Translational temperature, and

(2) Heavy particle Translational - Rotational temperature.

Ref.[1] presents the conservation laws for such a flow, considering 11 possible chemical species:

$$N, O, N_2, O_2, NO, N^+, O^+, N_2^+, O_2^+, NO^+, e^-$$

These equations are:

Species Conservation:

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u^j}{\partial x^j} = \frac{\partial (\rho D_s \frac{\partial y_s}{\partial x^j})}{\partial x^j} + w_s \quad (1)$$

Mixture Momentum Conservation:

$$\frac{\partial \rho u^i}{\partial t} + \frac{\partial \rho u^i u^j}{\partial x^j} = -\frac{\partial p}{\partial x^i} + \frac{\partial}{\partial x^j} \left[\mu \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right) - \frac{2}{3} \mu \frac{\partial u^k}{\partial x^k} \delta^{ij} \right] \quad (2)$$

Vibrational-Electronic Energy Conservation:

$$\frac{\partial \rho e_V}{\partial t} + \frac{\partial \rho e_V u^j}{\partial x^j} = -p_e \frac{\partial u^j}{\partial x^j} + \frac{\partial}{\partial x^j} \left[\eta_V \frac{\partial T_V}{\partial x^j} \right] + \frac{\partial}{\partial x^j} \left(\rho \sum_{s=1}^{11} h_{V,s} D_s \frac{\partial y_s}{\partial x^j} \right) \quad (3)$$

$$+ \sum_{s=mol.} \rho_s \frac{(e_{v,s}^* - e_{v,s})}{\langle \tau_s \rangle} + 2\rho_e \frac{3}{2} \bar{R}(T - T_V) \sum_{s=1}^{10} \frac{\nu_{es}}{M_s} - \sum_{s=6}^{10} n_{e,s} \hat{I}_s + \sum_{s=mol.} w_s \hat{D}_s - Q_{rad}$$

Total Energy Conservation:

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho H u^j}{\partial x^j} = \frac{\partial}{\partial x^j} \left(\eta \frac{\partial T}{\partial x^j} + \eta_V \frac{\partial T_V}{\partial x^j} \right) + \frac{\partial}{\partial x^j} \left(\rho \sum_{s=1}^{11} h_s D_s \frac{\partial y_s}{\partial x^j} \right) + \frac{\partial}{\partial x^j} \left[u^i \mu \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right) - \frac{2}{3} u^i \mu \frac{\partial u^k}{\partial x^k} \delta^{ij} \right] \quad (4)$$

Where:

ρ_s	Species density
u^j	Velocity vector
x^j	Position vector
t	time
ρ	Total density
D_s	Species diffusion coefficient
y_s	Species mole fraction
w_s	Species production rate
p	Pressure
μ	Mixture viscosity
e_V	Vibrational-electronic energy
p_e	electron pressure
η_V	Vibrational thermal conductivity
η_e	Electronic thermal conductivity
$h_{V,s}$	Species vibrational enthalpy
$e_{v,s}^*$	Vibrational energy at temperature T
$e_{v,s}$	Species vibrational energy
$\langle \tau_s \rangle$	Translational-Vibrational relaxation time
\bar{R}	Universal gas-constant
T	Translational-rotational temperature
T_V	Vibrational-Electronic temperature
ν_{es}	Species-electron collision frequency
$n_{e,s}$	Rate of production by impact ionization
Q_{rad}	Radiative energy transfer rate
I_s	Ionization energy
E	Total energy
H	Total Enthalpy
h_s	Species enthalpy

The physical phenomena that the above model describes are:

- (a) A total of 43 possible chemical reactions among the 11 species, (with the appropriate gas chemistry setup),
- (b) Diffusion of species,
- (c) Energy exchange (relaxation) between the two temperatures, and
- (d) Energy transfer in electron impact ionization,

Magnetohydrodynamics

The code is intended to simulate a nonequilibrium plasma entering the nozzle. Since high temperature air has large values of conductivity, it can be further accelerated by means of a magnetic field jointly with an electric field perpendicular to it. This necessitates the inclusion of Magnetohydrodynamic (MHD) terms in the fluid model. In order to accommodate for the MHD terms, the following assumptions are made:

(a) The Magnetic Reynolds number $Re_m = \mu_0 \sigma_0 V_0 L_0$ is very small.

(b) Ion-Slip is negligible, and there is no charge separation.

Assumption (a) permits the decoupling of the fluid equations and the electrodynamic equations. The magnetic Reynolds number is representative of the amount of induced magnetic field generated in the flow. By assuming it to be zero, the electrodynamic equations can be reduced to a system of linear equations that can be solved independent of the flow equations. Let us start by detailing a quasi-one-dimensional flow situation. From Ref.[12], the equations governing such a flow are:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho A \\ \rho u A \\ E_t A \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho u A \\ (\rho u^2 + p) A \\ (E_t + p) \rho u A \end{bmatrix} \quad (5)$$

$$= \begin{bmatrix} 0 \\ p dA/dx + J_y B_z \\ \mathbf{J} \cdot \mathbf{E} \end{bmatrix}$$

The source term contains contributions due to the electric field \mathbf{E} and the magnetic field \mathbf{B} that are applied. For several spatial dimensions, the current density \mathbf{J} is obtained from Ohm's law, in the following manner:

$$\mathbf{J} = \sigma (\mathbf{E} + \mathbf{V} \times \mathbf{B}) - \frac{\beta}{B} (\mathbf{J} \times \mathbf{B}) \quad (6)$$

The first term above is Ohm's law for an applied field. The second term comes from the Hall current. The scalar equations corresponding to the above law are:

$$J_x = \frac{\sigma}{1 + \beta^2} (E_x - \beta(E_y - uB)) \quad (7)$$

$$J_y = \frac{\sigma}{1 + \beta^2} (E_y - uB + \beta E_x)$$

Where E_x, E_y denote the components of the electric field \mathbf{E} and J_x, J_y denote the components of the current density. For multidimensional space, the electric field may be derived from a scalar potential, as:

$$\mathbf{E} = -\nabla \phi$$

Further, if the magnetic field is assumed to be along the z-direction, the current density can be written as:

$$J_x = \bar{\sigma} (-\phi_x + \beta \phi_y + \beta u B) \quad (8)$$

$$J_y = \bar{\sigma} (-\beta \phi_x - \phi_y - u B)$$

$$J_z = -\bar{\sigma} \phi_z$$

where $\bar{\sigma} = \sigma / (1 + \beta^2)$.

Conservation Laws and Flux Vectors

The governing equations of nonequilibrium flow stated earlier may be expressed more compactly in matrix form as:

$$\iiint \frac{\partial \mathbf{q}}{\partial t} d\Omega + \iint \bar{\mathbf{f}} \cdot \bar{\mathbf{n}} d\sigma = \iiint \omega d\Omega \quad (9)$$

where $\mathbf{f} = \mathbf{g} + \mathbf{h}$, is the net flux across a given control volume and \mathbf{g} and \mathbf{h} denote the inviscid and viscous fluxes respectively. The term ω on the right hand side denotes the source term, consisting of the production rates of each species and the vibrational energy. Additions can be made to this term to include an MHD force in the momentum equation and the Joule heating term in the energy equation.

The vector of conserved variables \mathbf{q} and the inviscid flux \mathbf{g} are:

$$\mathbf{q} = \begin{bmatrix} \rho_s \\ \rho u \\ \rho v \\ \rho E \\ \rho e_V \end{bmatrix} \quad \mathbf{g} = \begin{bmatrix} \rho_s U \\ \rho U u + p n_x \\ \rho U v + p n_y \\ \rho U H \\ \rho U e_V \end{bmatrix} \quad (10)$$

where U is the velocity normal to a face: $U = un_x + vn_y$. The viscous flux \mathbf{h} and the source term ω are:

$$\mathbf{h} = \begin{bmatrix} \rho D_s \frac{\partial y_s}{\partial s_n} \\ -\tau_{nx} \\ -\tau_{ny} \\ \left(-u\tau_{nx} - v\tau_{ny} - \eta \frac{\partial T}{\partial s_n} - \eta_V \frac{\partial T_V}{\partial s_n} - \rho \sum h_s D_s \frac{\partial y_s}{\partial s_n} \right) \\ -\eta_V \frac{\partial T_V}{\partial s_n} - \rho \sum h_{V,s} D_s \frac{\partial y_s}{\partial s_n} \end{bmatrix} \quad (11)$$

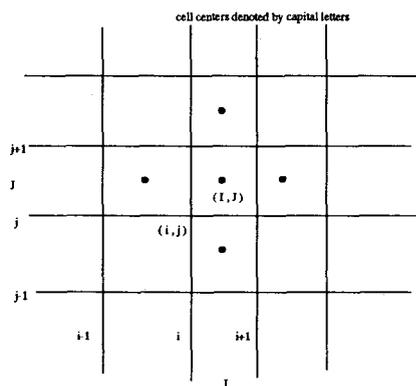


Figure 1: Cell geometry

$$\omega = \begin{bmatrix} \omega_s \\ 0 \\ 0 \\ Q_{rad} \\ \omega_V \end{bmatrix} \quad (12)$$

The cell geometry used for these computations is typified in Fig.[1]. The cell centers are denoted by upper case and grid indices are denoted by lower case letters. A generic index l and L are used to denote an arbitrary cell face and cell center respectively. The metric used to convert derivatives from x-y coordinates to $\xi - \eta$ coordinates using the thin layer assumption is :

$$\eta_n = \nabla \eta \cdot \vec{n} \quad (13)$$

This is the gradient of the variable η normal to a cell face whose unit normal is denoted by \vec{n} and has the components n_x and n_y .

In order to construct these fluxes and their Jacobian matrices with respect to the vector \mathbf{q} , they need to be redefined in terms of the elements of \mathbf{q} . If the elements of \mathbf{q} are numbered q_1 through q_{15} corresponding to the 11 species densities, 2 momenta and 2 elements corresponding to the total energy and the vibrational energy, the elements of \mathbf{g} and \mathbf{h} can then be written in terms of q_i .

The inviscid flux \mathbf{g} is easily expressed in terms of \mathbf{q} as follows:

$$\begin{aligned} i = 1 - 11, g_i &= q_i \left[\frac{q_{12}}{\sum q_k} n_x + \frac{q_{13}}{\sum q_k} n_y \right] \\ g_{12} &= q_{12} \left[\frac{q_{12}}{\sum q_i} n_x + \frac{q_{13}}{\sum q_i} n_y \right] + p n_x \\ g_{13} &= q_{13} \left[\frac{q_{12}}{\sum q_i} n_x + \frac{q_{13}}{\sum q_i} n_y \right] + p n_y \end{aligned} \quad (14)$$

$$\begin{aligned} g_{14} &= (q_{14} + p) \left[\frac{q_{12}}{\sum q_i} n_x + \frac{q_{13}}{\sum q_i} n_y \right] + p \\ g_{15} &= q_{15} \left[\frac{q_{12}}{\sum q_i} n_x + \frac{q_{13}}{\sum q_i} n_y \right] \end{aligned}$$

This flux is easily differentiated with respect to \mathbf{q} and the ensuing Jacobian matrix is listed under:

$$\mathbf{A} = \begin{bmatrix} U(\delta_{sr} - c_s) & c_s n_x & c_s n_y \\ \gamma_r n_x - Uu & un_x(1 - \beta) + U & -\beta v n_x + v n_y \\ \gamma_r n_y - Uv & -\beta u n_y + v n_x & v n_y(1 - \beta) + U \\ \gamma_r U - UH & -\beta u U + H n_x & -\beta v U + H n_y \\ -Ue_V & e_V n_x & e_V n_y \\ 0 & 0 \\ \beta n_x & \phi n_y \\ \beta n_y & \phi n_x \\ \beta U + U & \phi U \\ 0 & U \end{bmatrix} \quad (15)$$

The implementation of an upwind-based scheme to solve the above conservation law also requires the values of the eigen values and the right and left eigen vectors for the above matrix. These have been derived to be:

$$\mathbf{R} = \begin{bmatrix} \frac{\delta_{sr}}{a^2} & 0 & \frac{c_s}{2a^2} & \frac{c_s}{2a^2} & 0 \\ \frac{u}{a^2} & l_x & \frac{u+an_x}{2a^2} & \frac{u-an_x}{2a^2} & 0 \\ \frac{v}{a^2} & l_y & \frac{v+an_y}{2a^2} & \frac{v-an_y}{2a^2} & 0 \\ \frac{\beta(u^2+v^2)-\gamma_r}{\beta a^2} & V & \frac{H+aU}{2a^2} & \frac{H-aU}{2a^2} & -\frac{\phi}{\beta a^2} \\ 0 & 0 & \frac{e_V}{2a^2} & \frac{e_V}{2a^2} & \frac{1}{a^2} \end{bmatrix}$$

and its inverse consists of the left eigen vectors. The diagonal matrix of eigen values for the above system is defined by:

$$\Lambda = \begin{bmatrix} U & 0 & 0 & 0 & 0 \\ 0 & U & 0 & 0 & 0 \\ 0 & 0 & U+a & 0 & 0 \\ 0 & 0 & 0 & U-a & 0 \\ 0 & 0 & 0 & 0 & U \end{bmatrix}$$

The partial derivatives of pressure that have been used in the above expression, are:

$$\begin{aligned} \beta &= \frac{\partial p}{\partial \rho E} = \frac{R}{\rho C_{v,tr}} \sum_{r \neq e} \frac{\rho_r}{M_r} \\ \phi &= \frac{\partial p}{\partial \rho e_V} = \frac{R}{\rho C_{v,v}} \frac{\rho_e}{M_e} - \beta \\ \gamma_s &= \frac{\partial p}{\partial \rho_s} = \frac{RT_q}{M_s} + \frac{\beta}{2}(u^2 + v^2) - \beta e_s - \phi e_{V,s} \\ a^2 &= \sum c_s \gamma_s + \beta[H - u^2 - v^2] + \phi e_V \end{aligned} \quad (16)$$

The numerical scheme uses the absolute values of the eigen values defined earlier, with constraints on the minimum allowed magnitude of an eigen value. These are determined as:

$$\lambda_i = \begin{cases} |\lambda_i|, & |\lambda_i| \geq 2\epsilon_l \\ \frac{|\lambda_i|^2}{4\epsilon_l} + \epsilon_l, & |\lambda_i| < 2\epsilon_l \end{cases} \quad (17)$$

where ϵ_l is defined at a cell interface as:

$$\epsilon_l = \epsilon_0(a_l + |U_l| + |V_l|)$$

with ϵ_0 is a small number usually chosen in the range of 0.01 to 0.3. The larger values of ϵ_0 are chosen for flows with extensive stagnation regions. This completes the definition of the inviscid fluxes.

The viscous flux is simplified by making the thin layer assumption, as per which, if ξ denotes the flow direction along a wall and η denotes the direction that is transverse to this direction, the derivatives with respect to ξ in the viscous flux are negligible compared to the derivatives with respect to η . The expressions for the shear stresses can then be written as:

$$\tau_{nx} = \mu_l \left[\frac{\partial u}{\partial \eta} + \frac{1}{3} \frac{\partial U}{\partial \eta} n_x \right] \eta_n \quad (18)$$

$$\tau_{ny} = \mu_l \left[\frac{\partial v}{\partial \eta} + \frac{1}{3} \frac{\partial U}{\partial \eta} n_y \right] \eta_n \quad (19)$$

Under the same assumption, the derivatives of a quantity along a direction s_n may be rewritten as:

$$\frac{\partial T}{\partial s_n} = \frac{\partial T}{\partial \eta} \eta_n \quad (20)$$

Using these approximations, the viscous flux \mathbf{h} can be written component-wise in the following manner:

$$\begin{aligned} i = 1 - 11, h_i &= -(\sum q_j) D_i \frac{\partial}{\partial \eta} \left[\frac{q_i/M_i}{\sum q_j/M_j} \right] \eta_n \quad (21) \\ h_{12} &= -\mu_l \left[\frac{\partial q_{12}/\sum q_j}{\partial \eta} \right. \\ &\quad \left. + \frac{n_x}{3} \frac{\partial}{\partial \eta} \left[\frac{q_{12}n_x + q_{13}n_y}{\sum q_j} \right] \right] \eta_n \\ h_{13} &= -\mu_l \left[\frac{\partial q_{13}/\sum q_j}{\partial \eta} \right. \\ &\quad \left. + \frac{n_y}{3} \frac{\partial}{\partial \eta} \left[\frac{q_{12}n_x + q_{13}n_y}{\sum q_j} \right] \right] \eta_n \end{aligned}$$

$$\begin{aligned} h_{14} &= \left[\frac{q_{12}}{\sum q_j} h_{12} + \frac{q_{13}}{\sum q_j} h_{13} - \right. \\ &\quad \left. \eta_n \left(\eta \frac{\partial T}{\partial \eta} + \eta_v \frac{\partial T_V}{\partial \eta} \right) \right. \\ &\quad \left. + (\sum q_j) \sum h_k D_k \frac{\partial}{\partial \eta} \left[\frac{q_k/M_k}{\sum q_j/M_j} \right] \right] \\ h_{15} &= -\eta_n \left[\eta_v \frac{\partial T_V}{\partial \eta} + (\sum q_j) \right. \\ &\quad \left. \sum h_{v,k} D_k \frac{\partial}{\partial \eta} \left(\frac{q_k/M_k}{\sum q_j/M_j} \right) \right] \end{aligned}$$

This equation set is made complete by defining the partial derivatives of the two temperatures T and T_V and enthalpies h and $h_{v,k}$ with respect to \mathbf{q} . These are derived from the differential relations for T and T_V :

$$\rho C_{v,tr} dT = \quad (22)$$

$$\frac{u^2 + v^2}{2} \sum d\rho_s - \sum (e_s - e_{v,s}) d\rho_s -$$

$$ud(\rho u) - vd(\rho v) + d(\rho E) - d(\rho e_V)$$

$$\rho C_{v,v} dT_V =$$

$$d(\rho e_V) - \sum e_{v,s} d\rho_s$$

The derivatives of h_s and $h_{v,s}$ can be computed by writing them in the form:

$$h_s = e_s + \frac{RT_s}{M_s} \quad (23)$$

$$h_{v,s} = e_{v,s}$$

The differential of the energies e_s and $e_{v,s}$ are expressed in terms of the differentials of the two temperatures:

$$de_s = C_{v,tr}^s dT + C_{v,v}^s dT_V \quad (24)$$

$$de_{v,s} = C_{v,v}^s dT_V$$

Letting the index s denote the species number, the derivatives of the enthalpies then work out to (for $s \neq 11$ and $j = 1 - 11$):

$$\frac{\partial h_s}{\partial q_j} = \left(\frac{R}{M_s} + C_{v,tr}^s \right) \frac{\partial T}{\partial q_j} + C_{v,v}^s \frac{\partial T_V}{\partial q_j} \quad (25)$$

$$\frac{\partial h_{v,s}}{\partial q_j} = C_{v,v}^s \frac{\partial T_V}{\partial q_j}$$

In the case of the electron species for which $s = 11$, the first expression above is rewritten as:

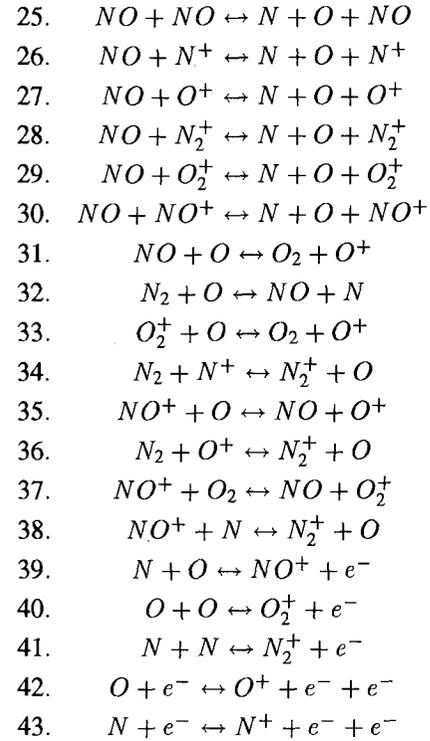
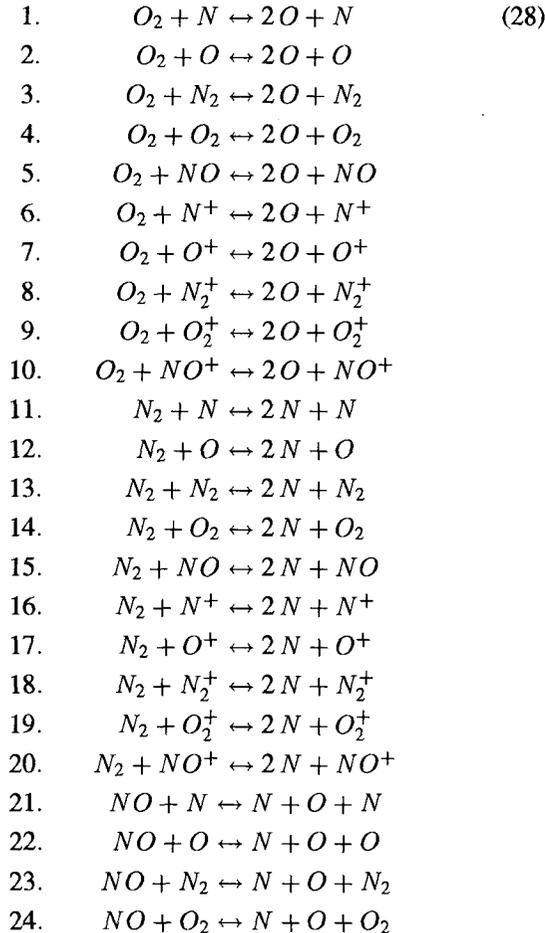
$$\frac{\partial h_{11}}{\partial q_j} = C_{v,tr}^s \frac{\partial T}{\partial q_j} + \left(\frac{R}{M_s} + C_{v,v}^s \right) \frac{\partial T_V}{\partial q_j} \quad (26)$$

Source Term and Jacobian

An implicit treatment of the source term in the present system of equations requires the evaluation of its Jacobian with respect to the vector \mathbf{q} . The source term consists of two types of entries, namely, the species production rate term (from chemical kinetics,) and the vibrational energy production rate term. For convenience, the vectors \mathbf{q} and the source term ω are:

$$\mathbf{q} = \begin{bmatrix} \rho_s \\ \rho u \\ \rho v \\ \rho E \\ \rho e_v \end{bmatrix} \quad \omega = \begin{bmatrix} \omega_s \\ 0 \\ 0 \\ Q_{rad} \\ \omega_v \end{bmatrix} \quad (27)$$

The various equations being considered in the present work are: (the collisional reactions in which the colliding species occurs in the same form on both sides of the equation are governed by the same rate law)



The production rate for a species with index s is:

$$\omega_s = M_s \sum_{r=1}^{N_r} (\beta_{s,r} - \alpha_{s,r}) [R_{f,r} - R_{b,r}] \quad (29)$$

where N_r is the total number of reactions being considered and $R_{f,r}$ and $R_{b,r}$ denote the rates of the forward and backward reactions for the reaction r . These are given by:

$$R_{f,r} = k_{f,r} \prod \left(\frac{\rho_k}{M_k} \right)^{\alpha_{k,r}}, \quad R_{b,r} = k_{b,r} \prod \left(\frac{\rho_k}{M_k} \right)^{\beta_{k,r}} \quad (30)$$

The quantities $k_{f,r}$ and $k_{b,r}$ are forward and backward reaction rate coefficients and are determined from empirical curve fits.

The term ω_s depends explicitly on species density and the two temperatures. The Jacobian of ω_s with respect to \mathbf{q} is evaluated by writing out the chain rule as:

$$\frac{\partial \omega_s}{\partial q_j} = \frac{\partial \omega_s}{\partial q_j} \Big|_{T, T_v} + \frac{\partial \omega_s}{\partial T} \Big|_{T_v, \mathbf{q}} \frac{\partial T}{\partial q_j} + \frac{\partial \omega_s}{\partial T_v} \Big|_{T, \mathbf{q}} \frac{\partial T_v}{\partial q_j} \quad (31)$$

It may now be noticed that the partial derivatives of ω_s can be computed from the partial derivatives of the reaction rates. Further, the reaction rate coefficients depend only on

the temperature and do not change the expressions for the derivatives with respect to the densities. The partial derivatives with respect to temperatures are contributed only by the reaction rate coefficients. These are written out explicitly as follows:

$$\begin{aligned}\frac{\partial R_{f,r}}{\partial \rho_s} &= k_{f,r} \prod \left(\frac{\rho_k}{M_k} \right)^{\alpha_{k,r}} \left(\frac{\alpha_{j,r}}{\rho_s} \right) \\ \frac{\partial R_{b,r}}{\partial \rho_s} &= k_{b,r} \prod \left(\frac{\rho_k}{M_k} \right)^{\beta_{k,r}} \left(\frac{\beta_{j,r}}{\rho_s} \right)\end{aligned}\quad (32)$$

The reaction rate coefficients are expanded as:

$$k_{f,r} = C_{f,r} T_q^{n_{f,r}} e^{-E_{f,r}/kT_q} \quad (33)$$

$$k_{b,r} = \frac{k_{f,r}}{K_{c,r}} \quad (34)$$

$$K_{c,t} = e^{B_1^r + B_2^r \log(Z) + B_3^r Z + B_4^r Z^2 + B_5^r Z^3} \quad (35)$$

$$Z = \frac{10000}{T_q} \quad (36)$$

All the quantities left undefined above are tabulated constants. The derivatives of the above with respect to temperatures work out to:

$$\frac{\partial k_{f,r}}{\partial T} |_{T_V, q} = \frac{k_{f,r}}{T} \left(n_{f,r} - \frac{E_{f,r}}{kT} \right) \quad (37)$$

$$\frac{\partial k_{b,r}}{\partial T} |_{T_V, q} = \frac{1}{K_{c,r}} \frac{\partial k_{f,r}}{\partial T} - \frac{k_{f,r}}{K_{c,r}^2} \frac{\partial K_{c,r}}{\partial T} \quad (38)$$

$$\begin{aligned}\frac{\partial K_{c,r}}{\partial T} &= K_{c,r} \left[\frac{B_2^r}{Z_r} + B_3^r + 2B_4^r Z + \right. \\ &\quad \left. 3B_5^r Z^2 \right] \left(\frac{-10000}{T^2} \right)\end{aligned}\quad (39)$$

The temperature used in the differentiation is temperature on which the reaction depends. It is the vibrational temperature for the two reactions involving electronic collisions and the translational temperature for all other reactions.

The vibrational energy production rate is given by:

$$\omega_V = \quad (40)$$

$$\sum_{mol} \omega_s D_s - \sum_{r=elec.imp.} (R_{f,r} - R_{b,r}) I_r + \quad (41)$$

$$\begin{aligned}&\sum \rho_s \frac{e_{v,s}^* - e_{v,s}}{\langle \tau_s \rangle} \\ &+ e \rho_e R(T - T_V) \sum_{s \neq e} \frac{\nu_{e,s}}{M_s} - p_e \nabla \cdot \vec{u}\end{aligned}$$

$$\begin{aligned}\frac{\partial \omega_V}{\partial q_j} &= \\ &\sum \frac{\partial \omega_s}{\partial q_j} D_s - \sum \frac{\partial (R_{f,r} - R_{b,r})}{\partial q_j} I_r + \\ &\frac{\rho C_{v,V}}{\tau_V} \frac{\partial (T - T_V)}{\partial q_j} \\ &+ 3 \rho_e R \left(\sum_{s \neq e} \frac{\nu_{e,s}}{M_s} \right) \frac{\partial (T - T_V)}{\partial q_j}\end{aligned}$$

The terms that do not appear in the derivative expressions are assumed to not contribute to the implicit formulation.

The Numerical Method

Using the notation described above, the finite volume formulation is expressed as:

$$\left[\frac{\delta \mathbf{q}}{\delta t} \right]_L + \sum_{l=i,j} [\mathbf{g}_{l+1} + \mathbf{h}_{l+1}] \sigma_{l+1} - [\mathbf{g}_l + \mathbf{h}_l] \sigma_l = \omega \Omega_L \quad (42)$$

This may be expressed in terms of an implicit relaxation scheme in the following manner:

$$\left[\mathbf{I} + \frac{\delta t}{\Omega_L} \mathbf{M}_L \right] \delta \mathbf{q}_L = \frac{\delta t}{\Omega_L} \mathbf{r}_L \quad (43)$$

where $\delta \mathbf{q}_L = \mathbf{q}_L^{n+1} - \mathbf{q}_L^n$ if n denotes the time level. In the above, \mathbf{I} denotes the identity matrix and \mathbf{M} denotes a point implicit approximation for the jacobians summed over all the cell faces and \mathbf{r} denotes the residual, or an explicit upwind based scheme to solve the same equations. (The current scheme for the face fluxes is similar to the Roe fluxes with the exception that the averaging of the quantities is based on the perfect gas Roe-averaging and does not satisfy Roe's property U [19] for nonequilibrium flows. They are written out in the following manner:

$$\mathbf{r}_L = - \sum_{l=i,j} [\mathbf{g}_{l+1} + \mathbf{h}_{l+1} \sigma_{l+1}] - [\mathbf{g}_l + \mathbf{h}_l] \sigma_l + \omega \Omega_L \quad (44)$$

$$\mathbf{M}_L = r_{f_{inv}} \mathbf{M}_{L,inv} + r_{f_{vis}} \mathbf{M}_{L,vis} - \Omega_L \mathbf{M}_{L,src} \quad (45)$$

where the subscripts *inv*, *vis* and *src* refer to the inviscid, viscous and source terms. The \mathbf{M} terms above are the summation of the flux jacobians over all the cell faces. They are evaluated in a point implicit manner, which is to say that if a term in the jacobian involves the derivative across a cell face, it will bear functional dependence only on the properties of

the current cell. The rf terms are relaxation factors, which are fine-tuned to optimize convergence for a given problem. Typically, their values are: $rf_{inv} > 1.5$ and $rf_{vis} > 1$. The time step δt above can be divided out and allowed to be infinity, thereby dropping the identity matrix in the implicit formulation. The scheme then reduces to a pure relaxation algorithm.

At each point, $\delta \mathbf{q}$ is obtained by inverting the above system, taking care not to allow spurious fluctuations caused by nonlinear initial behaviour of the solution process. More details on this formulation can be obtained from ref.[18].

Each time that $\delta \mathbf{q}$ is computed, the two temperatures need to be updated to be consistent with the new value of \mathbf{q} . The temperatures are updated using a Newton-Raphson scheme given by :

$$T^{k+1} = T^k + \frac{e - \sum \rho_s e_s}{\rho C_{v,tr}} \quad (46)$$

$$T_V^{k+1} = T_V^k + \frac{\rho e_V - \sum \rho_s h_{V,s}}{\rho C_{v,V}} \quad (47)$$

where e and e_V are the internal energy and the vibrational energy obtained from the updated \mathbf{q} vector. The superscript k denotes the Newton-Raphson iteration step. The individual e_s and $e_{V,s}$ for each species are dependent on the temperatures, and change with the current value of temperature. The iteration is carried out until convergence is attained to some level of tolerance ($10^{-4}K$).

The time accuracy in the above is achieved by means of subiterations between time levels, using a Runge-Kutta time stepping, as described in Refs. [20] and [21]

PRELIMINARY RESULTS

This method has been coded and is being tested for various geometries. The code is designed to run on workstations for reasonably small grid sizes. The first case studied is a wedge flow at a Mach number of approximately 3, at a free stream temperature of 3000 K and density of 1.2 kg/m^3 . Both the translational and vibrational temperatures are initially constant and evolve as solution progresses. Supersonic inflow and outflow boundary conditions are assumed. An adiabatic wall boundary condition is used for both temperatures. The wall is also assumed to be completely non-catalytic. Hence the species densities have zero gradients normal to the wall. No-slip boundary condition is imposed at the wall by setting the velocity in the ghost cells to the negative of the velocity of the cells immediately above the wall. Figs. [2] - [5] show preliminary results in this case.

The contours of translational and vibrational temperatures are plotted in Figs. [2] and [3] respectively. Fig. [4] shows

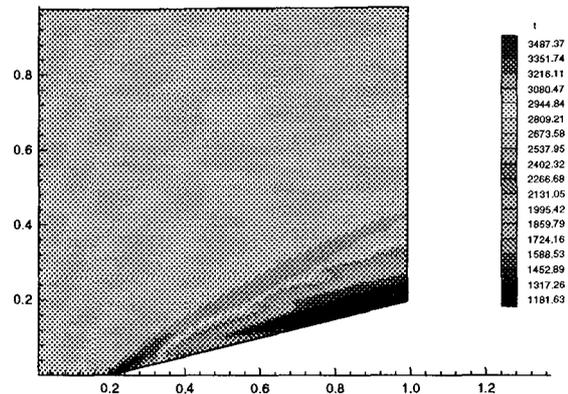


Figure 2: Translational temperature contours

the variation of these temperatures along a streamline near the stagnation region. The translational temperature is seen to rise immediately after the shock and fall rapidly, losing energy to the vibrational temperature. The trends of the nonequilibrium properties seem to be in the right direction. The details of these flow fields and their convergence properties are currently being investigated. Fig. [5] shows the variation of species concentrations along a streamline close to the wedge. The free stream was assumed to be composed of Nitrogen and Oxygen and trace amounts of the other species.

CONCLUSION

This work represents an initial phase in the development of unsteady nonequilibrium MHD based simulations. The code is intended to be applied to MHD augmented devices such as ground based wind tunnels as well as proposed dual mode propulsion systems. The equations being stiff, the time step constraint is overcome by making the numerical scheme implicit. The point implicit relaxation strategy that is being utilized is simple in concept. There are several parameters that may be manipulated in the present formulation to suit the specific type of problems solved. There are several issues of concern regarding the application of boundary conditions that would be appropriate for the MHD related cases. An isothermal wall and a catalytic wall boundary conditions are often found suitable for the intended applications. It is yet unknown as to the amount of stiffness caused by the addition of MHD terms to these equations. Future work involves incorporating these details in the current code.

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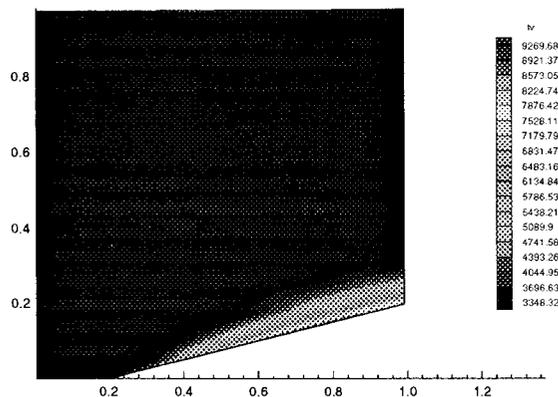


Figure 3: Vibrational temperature contours

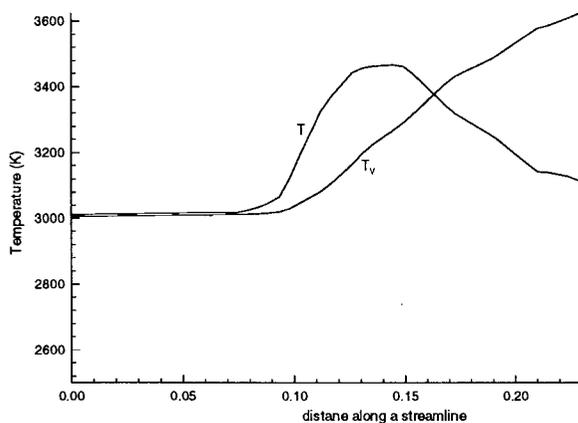


Figure 4: Variation of T and T_V through the shock

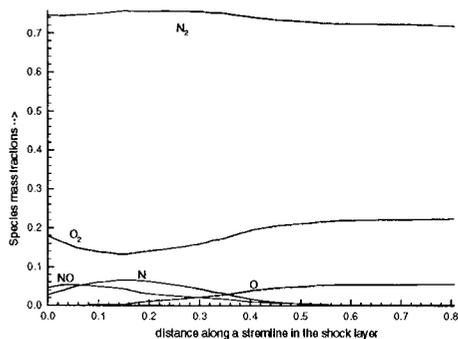


Figure 5: Concentration profiles along a streamline

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