DEVELOPMENT OF A THERMO-CHEMICAL NON-EQUILIBRIUM SOLVER FOR WEAKLY IONIZED HYPersonic FLOWFIELDS

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Abstract

A three dimensional solver for numerical simulation of weakly ionized hypersonic reactive air flows past high speed flight vehicles had been indigenously developed. The two-temperature, seven species, eighteen reactions, thermo-chemical non equilibrium, ionizing, air-chemistry model of Park is implemented in a compressible viscous code CERANS and solved in the finite volume framework. The energy relaxation is addressed by a conservation equation for the vibrational-electron-electronic energy of the gas mixture resulting in the evaluation of its vibrational temperature. The contribution of vibrational-electron-electronic energy of the reactive mixture is accounted in total energy equation as well as in the source terms of the relaxation model. The AUSM-PW+ numerical flux function has been used for modeling the convective fluxes and a central differencing approximation is used for modeling the diffusive fluxes. The code has been characterized for standard test cases involving weakly ionized hypersonic reactive thermo-chemical non equilibrium flows and results obtained are in good qualitative agreement with results available in open literature.

Keywords: CERANS solver, Air-chemistry, Weakly ionized flow, Hypersonic, Park’s model, Characterization

Nomenclature (SI Units)

\[ A = \text{Area of surface} \]
\[ A_s, B_s, C_s = \text{Blottner model constants} \]
\[ c_s, c_v = \text{Mass fraction of species} \]
\[ C_v = \text{Specific heat at constant volume} \]
\[ C_p = \text{Specific heat at constant pressure} \]
\[ D_s = \text{Species mass diffusion coefficient} \]
\[ e = \text{Specific energy} \]
\[ e_{ve} = \text{Specific vibrational-electron electronic energy} \]
\[ E_{ve} = \text{Total vibrational-electron energy} \]
\[ F_{\rightarrow j} = \text{Flux vector in the } j^{th} \text{ direction} \]
\[ g_{i,s} = \text{‘i’ th level electronic degeneracy of a species} \]
\[ h_s = \text{Total enthalpy of species} \]
\[ h_0^s = \text{Enthalpy of formation of species at 0K} \]
\[ I_s = \text{Mass diffusion species} \]
\[ j_{i,j} = \text{Mass diffusion of the } j^{th} \text{ species along the } i^{th} \text{ direction} \]
\[ k_{f}, k_{b} = \text{Forward and backward reaction rate coefficient} \]
\[ k_{eq} = \text{Equilibrium constant} \]
\[ L_e = \text{Lewis Number} \]
\[ M_s, M = \text{Molecular weight of the species} \]
\[ M_s, M_{sr} = \text{Number of Species} \]
\[ n_j = \text{Component of surface outward normal} \]
\[ N_{s} = \text{Number density of species} \]
\[ N_{av} = \text{Avagadro Number} \]
\[ p = \text{Pressure} \]
\[ p_s = \text{Partial pressure of species} \]
\[ p_e = \text{Partial pressure of electron} \]
\[ q_i = \text{Heat flux along } i^{th} \text{ direction} \]
\[ R_s = \text{Gas constant of the species} \]
\[ R_u = \text{Universal gas constant, 8314.34 J/kmol .K} \]
\( t \) = Time in seconds  
\( T \) = Translational temperature  
\( \bar{T} \) = Average temperature  
\( U \) = Conserved variable vector  
\( U_n \) = Contra-variant velocity  
\( V \) = Volume of cell element  
\( u, v, w \) = Velocity components along \( x, y, z \) directions  
\( x, y, z \) = Cartesian coordinate directions  
\( X_s \) = Mole fraction of species  
\( \gamma \) = Ratio of specific heats  
\( \delta_{ij} \) = Kronecker delta  
\( \theta_d \) = Dissociation temperature  
\( \theta_{el,i,s} \) = Characteristic electronic temperature of a species  
\( \theta_{vs} \) = Characteristics vibrational temperature of a molecular species  
\( \kappa \) = Thermal conductivity of the gas  
\( \mu \) = Coefficient of molecular viscosity of the gas  
\( \mu_s \) = Coefficient of molecular viscosity of species  
\( \rho_i \) = Density of \( i \)th species  
\( \tau_{ij} \) = Viscous shear stress  
\( \tau_s \) = Relaxation time  
\( \phi_s \) = Transport property model parameter  
\( \omega \) = Transport property model parameter  
\( \omega_p \) = Plasma frequency  
\( \omega_\rightarrow \) = Source term vector  
\( <> \) = Molar average  
1 \( atm \) = At 1 atmosphere  
\( fr, br \) = Forward reaction, backward reaction  
\( (i) \) = Inviscid  
\( i, j, k \) = Running index for Cartesian coordinate directions  
\( LT \) = Landau-Teller  
P = Park  
\( r, s \) = Reaction, species  
\( shock \) = Parameter at shock location  
\( t, r, v \) = Translational, rotational and vibrational energy modes  
\( vib \) = Vibrational energy mode  
\( vs \) = Vibrational species  
\( ve \) = Vibrational-electron electronic  
\( (v) \) = Viscous  

**Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CERANS</td>
<td>Compressible Euler/Reynolds Averaged Navier-Stokes solver</td>
</tr>
<tr>
<td>TCNEQ</td>
<td>Thermo-Chemical Non-EQuilibrium</td>
</tr>
<tr>
<td>LeMANS</td>
<td>Le Michigan Aerothermodynamic Navier Stokes solver</td>
</tr>
<tr>
<td>DPLR</td>
<td>Data Parallel Line Relaxation, CFD tool</td>
</tr>
<tr>
<td>VSL</td>
<td>Viscous Shock Layer code</td>
</tr>
<tr>
<td>AUSM-PW+</td>
<td>Advection Upstream Splitting Method with improved Pressure based Weights</td>
</tr>
</tbody>
</table>

**Introduction**

Hypersonic flight vehicles and spacecrafts during reentry possess large kinetic and potential energy due to its speed and altitude. This kinetic energy is converted into heat due to the formation of the strong detached shock and hence the vehicle experiences extreme flight conditions such as large temperature rise across the shock with a resultant severe heat flux on the surface. Depending on the flight altitude, Mach number and nose bluntness of the flight vehicle, the flow can be in a state of both chemical and thermal non equilibrium due to the physical and chemical processes occurring in the flow field such as vibration, dissociation, ionization and recombination of the constituent molecular species of the air. In many situations, the temperature on the surface of the vehicle is sufficient enough to ionize and ablate the heat shield material. This results in the formation of very complex mixture of ionized layer around the vehicle having constituents such as ionized air species called as plasma sheath. Due to large variations in plasma density and time scales associated with the plasma flow, the problem is not amenable for any analytical treatment. Also this complex phenomenon cannot be modeled in the routinely used CFD codes [1] typically applied for aerodynamic characterization as they are generally tailor made for calorically perfect gases in case of low speed flows and thermally perfect gases for high speed flows. Also ground testing for such flows with high enthalpy test facilities involving very high Mach number and altitude conditions are not an easy task and are not as routinely done as in case of the supersonic or low hypersonic test facilities. In many cases, the data generated at ground test facilities are directly extrapolated for the flight condition, therefore the test data have to be used with great prudence.
Hence it is necessary to develop a special purpose and reliable numerical prediction tool for simulation of such complex flows which are weakly ionized and are in chemical and thermal non-equilibrium. Development of such a capability is a prerequisite for optimally designing the thermal protection system, determination of range of communication blackout frequency with the flight communication system as well as for possible flow control by exploiting the electrical conductivity of the medium with suitable application of magnetic fields. It is in this realm that a CFD code namely, CERANS-TCNEQ [2] had been developed and characterized for standard non-ionizing thermo-chemical non-equilibrium test cases available in literature. This capability had been presently extended for modeling the weakly ionizing flows and the paper brings out an account of the various models used for modeling the complex physics, the numerical methods and characterization for standard test cases.

Necessity for Modeling the Plasma Flow

Due to very high temperature of gas behind the strong shock enveloping a reentry vehicle, the flow could be in a partially ionized gaseous state, also called as plasma. In a plasma flow, free electrons and ions are present in the flow field and hence it becomes an electrically conducting medium. The ionized gas forms a plasma layer between the shock envelope and the flight vehicle surface and is referred to as the plasma sheath. The formation and concentration of electrons and ions in the plasma sheath strongly depends on the reentry flight conditions, geometry of the vehicle, as well as the surface catalytic property of the airframe material that forms the heat shield. The number density of electrons and ions in the flowfield around the vehicle vary significantly and the flow may be electrically non-neutral. The gas which is composed of neutral species, free electrons and ions shall be in a state where there is a significant imbalance in the positive and negative charges giving rise to an electric field of sufficient magnitude so as to drag a neutralizing cloud of electrons in to the positively charged region [3]. Also the electrons oscillate in the plasma in order to preserve the macroscopic charge neutrality. The frequency of oscillation of electrons in the plasma sheath about a mean position is referred to as the electron-plasma frequency. Determination of the electron-plasma frequency for variety of flight conditions covering critical phases of the trajectory is an important aspect of the reentry flight vehicle design. When the electron plasma frequency coincides or exceeds the electromagnetic wave frequency of the radio frequency waves from the telemetry system, then the radio frequency waves gets attenuated causing severe decrease in its signal strength or a complete loss of signal, usually referred to as the ‘communication blackout’ or ‘reentry blackout’. Since the ground stations, GPS satellites as well as the flight vehicle are required to communicate continuously for signal communication and navigation, a blackout can lead to loss of real-time monitoring of the flight vehicle, which is a foremost requirement from the point of view of flight safety. This is very critical in case of manned space vehicles, where the loss of voice communication and telemetry data could be detrimental for the onboard crew as well as the mission. In case of reentry of ballistic missiles, a blackout could lead to loss of valuable electronic countermeasure capability. In order to alleviate or mitigate the problems associated with the presence of plasma sheath as well as to utilize it for flow controls, it is necessary to develop a capability to model and study the ionized reentry flows which can predict the electron number density, on which various parameters such as the electron-plasma frequency as well as the electrical conductivity of the medium depends upon.

The electron-plasma frequency ($\omega_p$) is a strong function of the electron number density and is given by

\[
\omega_p = \sqrt{\frac{N_e q_e^2}{\varepsilon_0 m_e}}
\]

where $N_e$ is the number density of electrons per cubic meter, $q_e$ is the electron charge, $\varepsilon_0$ is the permittivity of the free space, and $m_e$ is the mass of the electron. Since all the parameters except $N_e$ are constants, the expression for electron-plasma frequency in terms of Hz can be simplified as

\[
f_p = \frac{\omega_p}{2\pi} = 9.0 \sqrt{N_e} \text{ (Hz)}
\]

Once the radio signal blackout boundary for a given trajectory is known, it is possible to work out a suitable blackout mitigation scheme [4].

Another important aspect of modeling the plasma flow is that the electrical conductivity of the flow can be effectively utilized for active flow controls by suitably imposing magnetic fields over the plasma. During ballistic reentry, it is necessary to decelerate the flight vehicle by suitable aero-braking mechanisms, so as to subject it to benign levels of oncoming heat loads. One of the most
promising methods being promulgated is the magnetohydrodynamic (MHD) flow control [5], wherein the Lorentz force generated when a magnetic field is applied on an electrically conducting medium is used for creating the additional axial force which decelerates the flight vehicle. There are several other possibilities [5] of utilizing the weakly ionized flows for realization of various flow controls. These are the main motivational aspects that necessitated the development and characterization of the CERANS-TCNEQ solver for reliable prediction of weakly ionized flows.

**Governing Equations and Ionization Model**

The system of equations modeled are 7 species continuity equations, one total mass conservation equation, 3 momentum equations and 2 energy equations, one for representing the total energy and another for the vibrational-electron-electronic energy conservation. In general, the total energy is partitioned into translational, rotational, vibrational and electronic modes and hence requires representation of separate energy equation for each of these modes. Several approximations are made for reducing the complexity in description of various energy modes [6] and some that are considered in the present implementation is discussed.

In case of non-ionizing thermo-chemical non-equilibrium flow model, the partition energy due to vibrational mode is represented by a separate vibrational energy conservation equation and its evaluation leads to determination of the vibrational temperature $T_v$ which describes the state of vibrational excitation of the mixture. Also the rotational energy mode is assumed equilibrated with the translational energy mode and hence can be evaluated from the total energy conservation equation. Such model which describes evaluation of two temperatures for representing translational-rotational and vibrational states is called the two-temperature model.

However, for modeling the ionization effects, the partition energy corresponding to the electronic mode needs to be defined. This requires a separate electron and electronic excitation energy conservation equation (6) and its evaluation leads to determination of the electronic temperature $T_e$ which describes the electronic state of the mixture. Such a model which requires evaluation of three unique temperatures for describing all the partition modes is called a three-temperature model. An alternative possibility is to consider the two-temperature framework within which the essence of energy partition due to electronic mode is built in. In this approach it is assumed that the electronic temperature equilibrates with the vibrational temperature and hence the electron-electronic energy equation is not solved. Justification for adopting two temperature model are described in detail in Ref. [6]. However, to include the electronic energy into account without solving a separate electron-electronic energy equation, the vibrational energy equation of the non-ionizing two temperature model is replaced by the vibrational-electron-electronic energy equation. In this equation, the effects of energy exchanges due to electrons are taken into account in the form of source terms. Also the vibrational-electron-electronic energy consists of the species electronic energy terms described by the characteristic electronic temperature and the degeneracy of various electronic energy levels.

The species considered in the seven species model are $N_2$, $O_2$, NO, N, O, NO$_2$ and $e^-$. The first five species are the neutral components of the air, the next two are the single component ion and free electron respectively. The governing fluid dynamic conservation equations used in the present work are the Navier-Stokes equation in the Cartesian frame and the vector form of the conservative equations are represented as

$$\frac{\partial U}{\partial t} + \nabla \cdot (\vec{F}^{(i)} - \vec{F}^{(v)}) = \vec{\Omega}_{cv}$$

(3)

where, the superscript $i$ represents the inviscid terms and $v$ represents the viscous terms. $\vec{\Omega}_{cv}$ represents the source terms of the chemical reactions and vibrational energy equations. The equation sets are defined for conservation of mass for the number of species ($ns$) considered along with a conservation of mass of gas mixture, three momentum conservation equations and two energy equations. The energy equations include modeling of the vibrational relaxation process and conservation of total of energy. The above description of conservation set of equations is referred to as ‘the two-temperature model’. The integral forms of above equations are

$$\int_V U dV + \int_{A(V)} (\vec{F}^{(i)} - \vec{F}^{(v)}) dA = \int_V \vec{\Omega}_{cv} dV$$

(4)

In the finite volume framework, the above equation in Cartesian form is represented by

$$\frac{dU}{dt} V + \sum_{A(V)} (\vec{F}^{(i)} - \vec{F}^{(v)}), \vec{n} dA = \vec{\Omega}_{cv} V$$

(5)
where, \( U \) is the conserved variable vector, \( A(V) \) is the surface enclosing the volume \( V \). The flux vector is denoted by, \( F \), \( \hat{n} \) is the outward normal vector of surface and \( A(V) \) and \( \hat{\Omega} \) are the source term vector.

The conserved variable, inviscid, viscous fluxes and source term vectors are defined [7] as

\[
\hat{U} = \begin{bmatrix} \rho_s \\
\rho \\
\rho_u \\
\rho e \\
\rho e_{ve} \end{bmatrix}
\]

\[
\hat{F}^{(i)} = \begin{bmatrix} \partial J_{sj} \cdot \hat{n} \\
0 \\
\tau_{ij} \cdot \hat{n} \\
\vec{T} - \hat{\tau} \cdot \hat{n} - \vec{q} \cdot \hat{n} \\
- \hat{J}_s h \cdot \hat{n} - \hat{q}_{ve} \cdot \hat{n} - \hat{J}_s e_{ve} \cdot \hat{n} \end{bmatrix}
\]

\[
\hat{\Omega} = \begin{bmatrix} \omega_{c,s} \\
0 \\
0 \\
\omega_{ve} \end{bmatrix}
\]

In the above equations, \( \rho \) is the density of the gas mixture, and \( \rho_1, \rho_2 \ldots \rho_n \) are the species densities, \( u, v, \ldots \) are the Cartesian velocity components, \( U_p \) is the contravariant velocity, \( \rho \) is the static pressure, \( e \) is the total energy per unit mass and \( e_{ve} \) is the vibrational-electron-electronic energy per unit mass. The subscript ‘ns’ corresponds to the number of species considered.

The viscous stresses are modeled using the Stokes’ hypothesis given by

\[
\tau_{ij} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{2}{3} \mu \left( \frac{\partial u_k}{\partial x_k} \right) \delta_{ij}
\]

(10)

where, \( \mu \) is the molecular viscosity of the mixture and \( \delta_{ij} \) is the Kronecker delta. The term \( u^T \) is the transpose matrix of velocity components and \( \vec{\tau} \) is the viscous stress tensor. The mass diffusive flux of each species’s is modeled using the Fick’s law of mass diffusion given by

\[
\vec{J}_{s \neq e} = \vec{I}_s - C_s \sum_{r \neq s} \vec{I}_r
\]

with

\[
\vec{I}_s = -\rho D_s \nabla C_s, \quad \text{and} \quad C_s, \text{the mass fraction of the species. Here} D_s \text{is the species mass diffusion coefficient.}
\]

The heat flux terms which defines the thermal diffusion is modeled using Fourier’s law of heat conduction given by

\[
\vec{q} = - (\kappa_c + \kappa_r) \frac{\partial T}{\partial \chi_k} - \kappa_{ve} \frac{\partial T_{ve}}{\partial \chi_k} + \sum_{s=1}^{ns} J_s h_s
\]

(11)

where, the total enthalpy is, \( h_s = e_s + R_s T \), \( T \) is the translational temperature, \( T_{ve} \) is the vibrational temperature, \( \kappa_r \) and \( \kappa_c \) are the thermal conductivities due to the translational and rotational energy modes, \( \kappa_{ve} \) is the thermal conductivity due to vibrational-electron-electronic mode and \( R_s \) is the species gas constant. In the present model electron temperature is assumed to be equilibrated with the vibrational temperature.

**Thermodynamic Relations**

The total energy for the two-temperature model [4] is given by
\[ \rho e = \sum_{\text{mol}} \frac{5}{2} \rho_s \frac{R_u}{M_s} T + \sum_{\text{atom}} \frac{3}{2} \rho_s \frac{R_e}{M_s} T + \sum \rho_s h_s^0 + \frac{1}{2}(u^2 + v^2 + w^2) + \sum \rho_s e_{ve,s} \]

(12)

The first two terms correspond to the translation-rotational energy per unit volume of the mixture gas, third term correspond to the formation enthalpy of the species corresponding to 0K, the fourth term correspond to the total kinetic energy of the mixture and the last term represent the sum of the total vibrational energy content of the mixture considered only for the molecular species and the electronic energy of the mixture considered for both the molecular and atomic species. The last term is defined as the vibrational-electron-electronic energy of the mixture or \( E_{ve} \).

The species vibrational energy and the electron electronic energy per unit volume is represented [7] as

\[ e_{ve,s} = \begin{cases} 
\varepsilon_s^{\text{vib}} & \text{for molecules and atoms} \\
\varepsilon_s^{el} & \text{for electrons}
\end{cases} \]

(13)

where

\[ \varepsilon_s^{\text{vib}} = \frac{R_u}{T_{ve}} \left( \frac{\theta_{vs}}{T_{ve}} - 1 \right) \]

for molecules

(14)

and

\[ \varepsilon_s^{el} = \sum_{i=1}^{\infty} \frac{R_u}{M_i} \sum_{s=1}^{ns} \frac{g_{i,s} \theta_{el,i,s} \exp(\theta_{el,i,s}/T_{ve})}{\exp(\theta_{el,i,s}/T_{ve})} \]

for molecules and atoms

(15)

In the above equation, \( \theta_{vs} \) is the characteristic vibrational temperature of the species and is provided in Table-1. The terms \( \theta_{el,i,s} \) and \( g_{i,s} \) correspond to the characteristic electronic temperature and the electronic degeneracy of the \( i \)-th energy level. The values of these parameters are available in Ref. [7].

**Equation of State**

The equation of state at thermal non equilibrium is given by the Dalton’s law of partial pressures which states that the pressure of the gas \( p \) can be expressed as sum of partial pressures of the individual participating species \( p_s \) with the assumption that the individual species behave as perfect gas. Apart from the molecules, atoms and ions, electrons contribute for the fluid pressure with the temperature governed by the vibrational state of the gas and the expression for pressure is

\[ p = \sum_{s=1}^{ns} p_s = \rho \sum_{s=1}^{ns} \frac{C_s}{M_s} + \rho_e \frac{R_e}{M_e} T_{ve} \]

(16)

**Modeling of Transport Properties**

The individual species viscosities are calculated using the curve fit model of Blottner [8] given by

\[ \mu_s = 0.1 \exp \left[ (A_s \ln (T) + B_s) \ln (T) + C_s \right] \]

(17)

<table>
<thead>
<tr>
<th>Species</th>
<th>( \theta_{vs} )</th>
<th>( A )</th>
<th>( B )</th>
<th>( C )</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2</td>
<td>3395</td>
<td>0.0268142</td>
<td>0.3177838</td>
<td>-11.3155513</td>
</tr>
<tr>
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<td>2239</td>
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<td>NO</td>
<td>2817</td>
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<td>-0.0335511</td>
<td>-9.5767430</td>
</tr>
<tr>
<td>N</td>
<td>0</td>
<td>0.0115572</td>
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<td>-12.4327495</td>
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<tr>
<td>O</td>
<td>0</td>
<td>0.0203144</td>
<td>0.4294404</td>
<td>-11.6031403</td>
</tr>
<tr>
<td>NO(^+)</td>
<td>2817</td>
<td>0.3020000</td>
<td>3.5039791</td>
<td>-3.7400000</td>
</tr>
<tr>
<td>e(^-)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-12.000000</td>
</tr>
</tbody>
</table>

Table-1 : Model Constants of Various Species
where $A_s$, $B_s$ and $C_s$ empirical constants given in Table-1.

The transport properties of the gas mixture is obtained using Wilke’s mixing rule [7] as

$$
\mu = \sum_{s=1}^{n_s} X_s \mu_s \phi_s
$$

(18)

and

$$
\kappa = \sum_{s=1}^{n_s} X_s \kappa_s \phi_s
$$

(19)

where $X_s$ is the mole fraction of the species, $\mu_s$ is the coefficient of viscosity of the species and $\kappa_s$ is the thermal conductivity of the species. $\phi_s$ is defined as

$$
\phi_s = \sum_{r=1}^{n_r} X_s \left[ \frac{1}{8 (1 + \frac{M_r}{M_s})^{1/2}} \right]
$$

(20)

where $M_s$ is the species molecular weight. The species thermal conductivities can be obtained using the Eucken’s relation [7] which is given for the translational-rotational mode as

$$
\kappa_{tr,s} = \frac{5}{2} \mu_s C_{v,t,s} + \mu_s C_{v,r,s}
$$

(21)

where $C_{v,t,s} = \frac{3}{2} R_s$ and for the vibrational mode as

$$
\kappa_{ve,s} = \mu_s C_{v,e,s}
$$

(22)

The vibrational mode thermal conductivity is considered only for the diatomic species. The individual species mass diffusion coefficient $D_s$ is considered to be same for all the species and it can be obtained by assuming constant Lewis number, using the relation, $D_s = \frac{D \cdot L_e \cdot \kappa}{(p C_p)}$, where $L_e$ is the Lewis Number equal to 1.4, $\kappa$ is the mixture translational-rotational thermal conductivity and $C_p$ is the mixture translational-rotational specific heat at constant pressure.

**Finite-Rate Chemical Kinetics Model**

During reentry of flight vehicles, depending on the flight conditions, the air molecules as it traverses through the detached shock, experience temperatures of the order of several thousands of degrees and therefore dissociate into atoms, ionize into various ions and recombine to form new species. Hence the air chemistry model should represent the evolution of relevant species depending on the gas temperature and the excitation of various energy levels.

For the ionizing flow model is considered in this work, the Park model [5] is used with 7 participating species namely, $N_2$, $O_2$, $NO$, $N$, $O$, $NO^+$ and $e^-$ with 18-reactions. The chemical reaction are generically represented as

$$
\sum_{s=1}^{n_s} \nu_s \cdot X_s \cdot \frac{k_{f,s}}{k_{b,s}} \sum_{s=1}^{n_s} \nu_s' \cdot X_s
$$

(23)

The source terms of species evolution equation is given by

$$
\omega_{cs} = \frac{M_s}{\sum_{r=1}^{n_r} \nu_s' - \nu_s'} J_r
$$

(24)

where

$$
J_r = 1000 k_{fr} \Pi s \left[ \frac{\rho_s^{\nu_s'}}{M_s} \right] - 1000 k_{br} \Pi s \left[ \frac{\rho_s^{\nu_s''}}{M_s} \right]
$$

(25)

Here, $\nu_s'$ and $\nu_s''$ are the stoichiometric coefficients equal to the stoichiometric mole numbers of the reactants and products respectively and the term $\left( \rho_s / M_s \right)$ is the molar density of the species. The terms $k_{fr}$ and $k_{br}$ are the forward and backward reaction rate coefficients. The factors 0.001 in the above equation converts [7] the species concentration from $kmol/m^3$ to $mol/cm^3$ and the factor 1000 converts $mol/cm^3/sec$ to $kmol/m^3/sec$, as reaction data are available in CGS unit system. The forward reaction rate coefficients are obtained using the Arrhenius equation of the form

$$
k_{fr}(T) = A_{fr} T^{\eta_f} \exp \left( - \frac{\theta_f}{T} \right)
$$

(26)
where \( A_f, T, \eta_f \) and \( \theta_d \) or each reactions of Parks’ model are tabulated in Table-2. The backward reaction rate coefficients are obtained using the forward rate coefficient and the equilibrium constant,

\[
k_{br}(T) = \frac{k_f(T)}{k_{eq}(T)}
\]

(27)

where

\[
k_{eq}(T) = \exp \left( \frac{a_1}{z} + a_2 + a_3 \ln z + a_4 z + a_5 z^2 \right)
\]

(28)

and \( z = \frac{10000}{T} \)

The constants \( a_1, \ldots, a_5 \) are given in Table-3 for all the reactions.

For flow having significantly excited vibration modes, the reaction rates of the chemical model gets affected appreciably by the level of non-equilibrium. In order to model the reaction rates of the source terms of the species conservation equations, the Park’s model uses an effective temperature that blends the translation/rotational temperature and the vibrational temperature by a geometric average \( \overline{T} \) and this effective temperature will be used according to the type of reaction considered. Table-2 provides the \( \overline{T} \) for various reactions.

It has to be noted that the model data for reaction rate-coefficients of various reactions involving air-species are sourced from experimental measurements for temperature up to 7000K and further extrapolated using curve-fits for higher temperatures. According to Park [7], these rate-coefficient data have large uncertainty especially beyond 10,000K and differ by about one order of magnitude when compared with experimentally measured data.

### Table-2 : Forward Reaction Rate Coefficients for the Park’s Model Ref.[7]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Third Body ( M_i )</th>
<th>( A_f (cm^3/mol.s) )</th>
<th>( \eta_f )</th>
<th>( \theta_d (K) )</th>
<th>( \overline{T} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R1 : N_2 + M \to 2N + M ) Dissociation</td>
<td>( N_2 ) ( \quad )</td>
<td>( 7.00 \times 10^{21} )</td>
<td>-1.6</td>
<td>113200 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O_2 ) ( \quad )</td>
<td>( 7.00 \times 10^{21} )</td>
<td>-1.6</td>
<td>113200 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( NO ) ( \quad )</td>
<td>( 7.00 \times 10^{21} )</td>
<td>-1.6</td>
<td>113200 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( N ) ( \quad )</td>
<td>( 3.00 \times 10^{22} )</td>
<td>-1.6</td>
<td>113200 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O ) ( \quad )</td>
<td>( 3.00 \times 10^{22} )</td>
<td>-1.6</td>
<td>113200 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td>( R2 : O_2 + M \to 2O + M ) Dissociation</td>
<td>( N_2 ) ( \quad )</td>
<td>( 2.00 \times 10^{21} )</td>
<td>-1.5</td>
<td>59500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O_2 ) ( \quad )</td>
<td>( 2.00 \times 10^{21} )</td>
<td>-1.5</td>
<td>59500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( NO ) ( \quad )</td>
<td>( 2.00 \times 10^{21} )</td>
<td>-1.5</td>
<td>59500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( N ) ( \quad )</td>
<td>( 1.00 \times 10^{22} )</td>
<td>-1.5</td>
<td>59500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O ) ( \quad )</td>
<td>( 1.00 \times 10^{22} )</td>
<td>-1.5</td>
<td>59500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td>( R3 : NO + M \to N + O + M ) Dissociation</td>
<td>( N_2 ) ( \quad )</td>
<td>( 5.00 \times 10^{15} )</td>
<td>0</td>
<td>75500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O_2 ) ( \quad )</td>
<td>( 5.00 \times 10^{15} )</td>
<td>0</td>
<td>75500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( NO ) ( \quad )</td>
<td>( 1.10 \times 10^{17} )</td>
<td>0</td>
<td>75500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( N ) ( \quad )</td>
<td>( 1.10 \times 10^{17} )</td>
<td>0</td>
<td>75500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( O ) ( \quad )</td>
<td>( 1.10 \times 10^{17} )</td>
<td>0</td>
<td>75500 ( (T_T T_v)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td>( R4 : N_2 + O \to NO + N ) Exchange</td>
<td>( - ) ( \quad )</td>
<td>( 6.40 \times 10^{17} )</td>
<td>-1.0</td>
<td>38400 ( T_T )</td>
<td></td>
</tr>
<tr>
<td>( R5 : NO + O \to O_2 + N ) Exchange</td>
<td>( - ) ( \quad )</td>
<td>( 8.40 \times 10^{12} )</td>
<td>0</td>
<td>19450 ( T_T )</td>
<td></td>
</tr>
<tr>
<td>( R6 : N + O \to NO^+ + e^- ) Dissociative Recombination</td>
<td>( - ) ( \quad )</td>
<td>( 5.3 \times 10^{12} )</td>
<td>0</td>
<td>31900 ( T_T )</td>
<td></td>
</tr>
</tbody>
</table>
### Chemical Reactions

The 7-species reaction model considered here consists of the following six reactions:

- **R1**: \( N_2 + M \rightarrow 2N + M \)
- **R2**: \( O_2 + M \rightarrow 2O + M \)
- **R3**: \( NO + M \rightarrow N + O + M \)
- **R4**: \( N_2 + O \rightarrow NO + N \)
- **R5**: \( NO + O \rightarrow O_2 + N \)
- **R6**: \( N + O \rightarrow NO^* + e^- \)

Here, \( M \) is the impacting body which can be any one of the five species. The reaction \( R1 \) to \( R3 \) are the heavy-particle impact dissociation reactions and the forward reaction rate depends on the vibrational excitation of the molecules. The reactions \( R4 \) and \( R5 \) are exchange reactions or the Zeldovich Reactions. The reaction \( R6 \) is the called the dissociative recombination reaction. Each reaction results in production of the species which can be represented as follows:

\[
R = k_{b2} \frac{\rho_N \rho_N \rho_m}{M_1 M_2 M_m} - k_{f1} \frac{\rho_{N_2} \rho_m}{N_2 M_m} \tag{29}
\]

\[
R = \sum_{m_e \in M} \left( k_{b3} \frac{\rho_N \rho_N \rho_m}{M_1 M_2 M_m} - k_{f2} \frac{\rho_{N_3} \rho_m}{N_3 M_m} \right) \tag{30}
\]

\[
R = \sum_{m_e \in M} \left( k_{b4} \frac{\rho_{NO} \rho_N \rho_m}{M_1 M_2 M_m} - k_{f3} \frac{\rho_NO \rho_m}{NO M_m} \right) \tag{31}
\]

\[
R = k_{b4} \frac{\rho_{NO} \rho_N}{M_1 M_2} - k_{f4} \frac{\rho_{N_2} \rho_NO}{M_2} \tag{32}
\]

### Energy Relaxation Model

The source terms [7] of the vibrational-electron-electronic energy conservation equation, \( \dot{\omega}_e \), models the sum of work done on electrons by electron pressure gradients, energy transfer rate between heavy particles and electrons considering both the electron-neutral collisions and electron-ion collisions and the production/destruction of the vibrational energy modeled as harmonic oscillators. It can be represented as

\[
\dot{\omega}_e = \sum_{r=r_e}^{\infty} \sum_{\sigma=\sigma_e}^{\infty} \frac{\rho_e N}{M_e} \left[ \frac{y^2}{\pi M_e} \right] \sum_{\sigma=\sigma_e}^{\infty} \frac{\rho_e N}{M_e} \sigma_e
\]
heavy particles and electrons. The term $\sigma_{ee}$ is the collision cross sections between electrons and the heavy particles for which a value of $10^{-20}$ m$^2$ is used in case of electron-neutral collisions and a value equal to

$$\sigma_{ee} = \frac{8 \pi}{27} \frac{k}{2} \frac{3}{T_v e} \ln \left[ 1 + \frac{9k}{4 \pi N e^6} \right]$$

is used for electron-ion collisions.

The third term is due to the net production rate of the vibrational energy. The last term is due to translational/rotational-vibrational energy exchange and it is modeled using the Landau-Teller (9,10) equation. Here, $\langle \tau_{LT}^s \rangle$ is the molar averaged Landau-Teller relaxation time and is given by

$$\langle \tau_{LT}^s \rangle = \frac{\sum_{r=1}^{n_s} X_r}{\sum_{r=1}^{n_s} X_r / \tau_{LT}^s}$$

and the inter-species Landau-Teller relaxation time is correlated by the semi-empirical formula of Millikan and White [9,10]. It is given as

$$\tau_{LT}^s = \frac{P_{lam}}{P} \exp \left[ A_s \left( T^{1/3} - 0.015 \mu_s^{1/4} \right) - 18.42 \right]$$

$$A_s = 1.16 \times 10^{-3} \mu_s^{1/2} \frac{4}{\theta_{vs}}$$

$$\mu_s = \frac{M_s M_r}{M_s + M_r}$$

In the above expression for vibrational energy source term, $T_{shock}$ is the post shock temperature at which the relaxation process is assumed to begin. It can be simply taken as the post normal shock temperature ahead of the leading nose of the geometry. The term $T_{ ve, shock}$ is the corresponding vibrational-electron electronic temperature at that location. This formula is valid from about 300K to 8,000K and for temperatures beyond 8,000K, the Millikan and White formula results in unrealistically small relaxation times [11] due to over-prediction of the collision cross-section. To remedy this problem, a correction is made to the relaxation time by adding a collision limited relaxation time $\tau_{LT}^s$. Hence the corrected relaxation time becomes

$$\tau_{LT}^s = \langle \tau_{LT}^s \rangle + \tau_{LT}^s$$

where

$$\tau_{LT}^s = \frac{1}{a_s \sigma_{LT}^s}$$

$$\sqrt{\frac{8 R}{\pi M_s}} \frac{T}{T_{shock}}$$

$$\sigma_s = 10^{-21} \left( \frac{50,000}{T} \right)^2$$

$$S_s = 3.5 \exp \left[ -\frac{\theta_{ve}}{T_{shock}} \right]$$

**CERANS-TCNEQ Code**

The 7-species, 18-reaction, two-temperature, air chemistry model for simulating weakly ionizing flows, had been implemented in CERANS-TCNEQ code, which is a general purpose CFD code developed by the authors for solving the compressible RANS equations in cell centered finite volume framework on sequential and parallel computers. The code is designed to be grid format independent and hence several structured and unstructured grid preprocessors have also been developed requiring treatment of different types of data structures for each of these grid types. The code can handle complex geometries involving both structured as well as unstructured polyhedral grids [12,13]. It had been extensively validated for studying its accuracy, robustness and range of applicability. Presently, implementation of TCNEQ model had not been coupled with the turbulence model and hence can solve for either inviscid or laminar hypersonic flows. Due to the implementation of TCNEQ with ionization model, the number of governing equations to be solved had increased to 13 from 6. In the present work the convective fluxes are modeled using the AUSM-PW+ numerical flux functions [14].
Higher Order Accuracy

Higher order spatial accuracy is obtained using the method of reconstruction. The interfacial flow gradients required for the evaluation of viscous stresses are obtained by using cell-centered weighted least squares method for structured grids. The viscous flow gradients at the interface are further corrected for avoiding the odd-even decoupling. Barth’s min-max limiter had been used for preserving monotonicity. For the present study, only structured grids were considered for simulations as the configurations considered for the characterization are geometrically simpler to generate structured grids.

Boundary Conditions

At the inflow or farfield boundaries, freestream flow parameters are specified. At the outflow boundary, zero gradients for all the flow variables using the values from upstream cell are specified. At wall boundaries, flow tangency condition is applied for inviscid flows and no-slip and adiabatic conditions are specified for viscous flows. In case of an isothermal wall condition, temperature on the wall is specified. The vibrational temperature is set equal to the translational temperature at the wall. For specifying non-catalytic wall boundary condition, the normal gradient of specie-mass fraction at the wall is set to zero and for a fully catalytic wall, the specie-mass fraction at the wall is set equal to that of the freestream value.

Verification of Sub-models in CERANS-TCNEQ

The process of verifying various sub-models at different stages of development involves checking of the implemented mathematical models and their outputs against several published data for ascertaining their functionality for the intended purposes. The sub-models are tested as either standalone routines or monitored as coupled/integrated modules. During the implementation of these models in CERANS-TCNEQ, the important model parameters were verified against the known/published literature. In this regard, Ref.[7] and Ref.[11] consists of vast details on air-chemistry models and are the prime references for the present work.

The transport properties obtained using Wilke’s mixing rule were verified against the well known Sutherland’s law of viscosity up to about 2000K. Similarly the translational-rotational thermal conductivity obtained using the Eucken’s relation was verified against the thermal conductivity obtained by using definition of Prandtl number. The variation of specific heats was compared with known thermally perfect specific heat data up to about 2500K. The variation of reaction rates with temperature of Park’s air-chemistry model have been checked and found to conform to the published literature.

During hypersonic flow evolution over blunt body, vibrational temperature had been carefully examined and observed to increase only when the O2 species first starts to undergo vibrational excitation and further dissociation. The temperature range at which O2 and N2 dissociate have been carefully monitored and always observed to occur around the well known documented temperature ranges. Also the evolution of electron/ion species was observed to occur only after the large scale dissociation of N2 and O2 species. The physical realizability constraint that the sum of mass of species equal to the total mass obtained from mass conservation equation have been observed to occur all through the temporal evolution.

In order to avoid coding errors, the structured coding approach of ‘C’ language have been extensively used. The governing equation for seven species and total mass, three momentum and two-temperature energy conservation equations were solved using edge based data structure. Various terms of the governing equation such as the source terms, transport properties, thermal properties and partition energies were computed in the preprocessing stage before each iteration and are stored and retrieved for use during reconstruction and temporal evolution. In computing the source terms of species mass and vibrational/vibrational electron-electronic energy equations, the chemical reactions, order-of-reactions, participating species for each reactions, Arrhenius equations and reduction of reactions were all implemented in a structured way to avoid coding/conceptual errors.

The CERANS-TCNEQ code had been verified to solve the intended mathematical models and is able to qualitatively reproduce not only the overall final results of established codes such as LeMANS [16] and DPLR [21] for standard test cases, but also observed to mimic the expected physical behavior at the discrete level and during temporal evolution as a result of correct implementation of various sub-models.
Characterization of CERANS-TCNEQ Solver for Ionizing Flows

Radio Attenuation Measurement-C II Configuration

Geometry, Grid and Simulation Details: In the 1960’s NASA conducted a series of hypersonic flight experiments called as the Radio Attenuation Measurement (RAM) program[15] for studying the communication blackout occurring during reentry of flight vehicles into the progressively denser atmosphere at satellite speeds. During the flight of RAM-C II configuration, the peak electron number density was measured at various locations on the body along the wall normal direction [16]. The RAM-C II configuration consists of a spherically blunted cone having a nose radius of 0.1524m, half-cone angle of 9° and a length of 1.3m. The schematic of geometry adapted from Ref.[15] is shown in Fig.1. It indicates the reflectometer and electrostatic probes at various locations of the body. The geometry of RAM-C II is shown in Fig.2. The freestream conditions for simulations are provided in Table-4. The flow is considered to be laminar for the simulations and the wall is assumed non catalytic referred usually as ‘non-catalytic wall’ or NCW. The volumetric fraction of freestream atmospheric species considered for simulations are N$_2$ of 76.8% and O$_2$ of 23.2% corresponding to molar fractions of 79.1% of N$_2$ and 20.9% of O$_2$ as used by Candler [21], et al.

The structured grid used for simulation is shown in Fig.3. It consists of 51x17x81 points, (41 points on the wall along axial length, 17 points along the circumference and 81 points away from the wall) amounting to about 64,000 hexahedral cells. This is an optimal grid size arrived after solving the problem in two more grids. Comparison of results was made with the results available from Ref.[16]. In this reference, numerical simulations were carried out using 11-species air-chemistry model with both vibrational-electron electronic equilibrium and (VEEE) non-equilibrium (VEENIQ). In the first case of Ref.[6], the vibrational-electronic temperature is in equilibrium with the electron translation temperature and hence a two temperature model had been used. In the other case, a separate equation for electron translational energy is solved to obtain the electron translational temperature and is therefore not in equilibrium with the vibrational-electronic temperature, which is also referred to as the three temperature model. The modeling due to CERANS-TCNEQ shall be considered equivalent to the first case, mentioned above.

Prediction of Two Temperatures: Typical simulation results in the form of vibrational temperature contours are shown in Fig.4 for the 61km case. It can be observed that the vibrational temperature achieved a peak of over 12,000 K just behind the shock location and rapidly equilibrates as the flow approaches near the stagnation region, reaching the specified isothermal condition of 1,200 K. The distribution of temperatures along the stagnation line is plotted in Fig.5 and 6 respectively for the 61km and 71km flight conditions.

The temperature distributions shown in these figures mimic the physical phenomenon captured in the region from shock to blunt-nose. For the 61km flight condition, the translational-rotational temperature sharply increases to about 18,000K within a finite distance from x=0.014m to x=0.0115m across the shock layer which prevails over 7 cell widths. This observation is in direct contrast to the well known shock thickness of the order of one cell-width in case of a perfect gas flow simulations. Across the shock layer thickness, due to the vibrational excitation and dissociation of the diatomic species along with ionization reaction, the vibrational temperature steadily increases and continues to increase further downstream of the shock before reaching a plateau region at 0.008m from the nose reaching a value of about 14,000K. Also it can be observed that the slope of vibrational temperature and hence its gradient in the shock region is lower than the gradient of translational-rotational temperature clearly depicting the strong interdependence of translational-rotational state of the gas on the vibrational excitation state across the shock and vice-versa.

In the post shock state, the vibrationally excited species consumes substantial amount of energy for further dissociation thereby resulting in reduction of the gas translational-rotational temperature. As the translational temperature decreases to an intermediate level of about 12,000K at 0.007m from nose, the vibrational temperature also begin to decrease. Further downstream, the two tem-

<table>
<thead>
<tr>
<th>Altitude, km</th>
<th>Mach Number</th>
<th>Velocity m/sec</th>
<th>Density kg/m$^3$</th>
<th>Temperature (K)</th>
<th>Wall Temperature, (K)</th>
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<td>61</td>
<td>23.9</td>
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<td>2.7216e-4</td>
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</tr>
<tr>
<td>71</td>
<td>25.9</td>
<td>7632</td>
<td>7.6808e-5</td>
<td>216</td>
<td>1200</td>
</tr>
</tbody>
</table>
temperatures decrease in a similar fashion in the spatial expanse from 0.007m and rapidly equilibrates as the flow approaches the nose stagnation region, reaching the specified isothermal condition of 1200 K. The predicted near wall stagnation translational-rotational temperature is about 1263K and the stagnation vibrational temperature is about 1296K. The peak value of translational-rotational and vibrational temperature profiles corresponding to the electron equilibrium simulation values of Ref.[16] are about 21,000K and 13,000K respectively and the corresponding shock location is from x=0.0155m to x=0.011m.

Similar observations can be made regarding the 71km altitude flight condition. In this case, the peak values of two-temperatures predicted by CERANS-TCNEQ are 18,500K and 12,500K as against data of Ref.16 of about 18,000K and 13,000K. The location of shock is at 0.0115m as against 0.0105m due to Ref.[16].

Remarks on Difference in Shock Location and Peak Temperature : For a code having several complex sub-models implemented for mimicking the complex physics of thermo-chemical non-equilibrium flows with weak ionization, there are bound to be differences in results when comparisons are made with a different code such as that of Ref.[16]. Broadly the difference between CERANS-TCNEQ and the code due to Ref.[16] is basically in the number of species modeled, which is 11 in Ref.[16] where each of the constituent species has an additional ionic counterpart. In the present approach the electronic non-equilibrium is not addressed, i.e., electronic temperature is in equilibrium with the vibrational temperature. Also the transport properties used in Ref.[16] were based on Gupta’s collision cross-section data which are valid for hypervelocity flows as high as 10km/sec as compared to the presently used Wilke’ mixing rule and Blottner’s curve fits which have uncertainties in properties beyond 10,000K.

From the description of the results, it can be clearly observed that several complex and competing physico-chemical mechanisms are involved in the thermo-chemical non-equilibrium flows and the numerical solution of such flows strongly depend on the applicability range of various sub-models used, which therefore makes validation of the TCNEQ codes a daunting and challenging task. In this realm, it is appropriate to address characterization of CERANS-TCNEQ in terms of qualitative comparisons of various relevant parameters with literature data for assessing the degree of correctness and overall functionality of the present code.

Despite these important differences in the sub-models, CERANS-TCNEQ is able to mimic the physical trend of the two-temperature variation across the shock-layer akin to the results available in standard literature.

Prediction of Electron Number Density : In order to obtain the blackout frequency of RAM-C II during reentry, it is necessary to determine the electron number density in the flowfield during the critical phase of flight. Also during the flight conditions of about 80km to 60km, an avalanche of electron flow is expected, creating plasma sheath around the flight vehicle. In case of RAM-C II reentry, the onset of blackout had been from about 81km and the recovery is observed below 30km and hence the flight regime considered in the present analysis are already in the communication black out phase. Thus the accuracy of measure of electron number density in this phase of flight is critical from the point of view of flight safety.

For these simulations, the peak electron number density along the axial direction is plotted in Fig.7 for the 61km flight and in Fig.8 for the 71 km flight. It can be observed that the peak electron number density varies by two orders across the axial length with the highest value of 1.26x10^{20}/m^3 occurring at the nose and gradually falling to 8.1x10^{18}/m^3 at the rearward end. Qualitative comparison with results of Ref.[16] show that the peak electron number density for the 61km altitude condition is of the order of 3.1x10^{19}/m^3 with both the VEEE and VEENE conditions. The lowest number density occurs at the rearward end with a value of 1.3x10^{16}/m^3 for the VEEE case and about 6.4x10^{17}/m^3 for the VEENE case. The flight measured peak electron number density data due to reflectometer and electrostatic probe measurement at a few locations are also depicted. The present data is qualitatively similar to the VEEE case of Ref.[16].

In case of the 71km altitude condition, the highest value of peak electron number density along the axial direction is about 3.4x10^{19}/m^3 occurring at the nose and reduces to about 2.9x10^{17}/m^3 at the rearward end. The peak value due to Ref.[16] for the 71km altitude case is about 8x10^{19}/m^3 for both VEEE and VEENE cases. The lowest is about 2.5x10^{17}/m^3 for the VEEE case and about 6.7x10^{17}/m^3 for the VEENE case. The CERANS-TCNEQ data is qualitatively similar to the VEEE case of Ref.[16], and the VEEE model is in fact an equivalent representation of the presently developed model.
From the above analysis, it can be observed that the predicted magnitude of peak electron number density along the axial direction is of the same order as that of the literature data and it can be concluded that the prediction has good qualitative agreement.

**Electron Number Density Along Stagnation Line**: The electron number density profiles along the stagnation line are plotted in Fig.9 and 10 for both the 61km and 71km altitude flight. Across the forebody bow shock, the electron number density increases due to the dissociative recombination or ionization reaction producing an avalanche of electrons. The electron number density profiles plotted in the logarithmic scale shows the value increasing to several orders of magnitude across the shock. The post-shock number density remains almost constant until nearer to the wall and it reduces at the wall by roughly one order for 61km case and by about half order for the 71km case due to the prevailing cold wall condition with wall temperature imposed at 1200K. Along with the present data, the results from Ref.16 are also plotted. The peak electron number density in case of Ref.[16] with VEENE simulation for 61km case is 1.9x10^{19}/m^3, which is very close to the present prediction. It can be observed that the overall qualitative agreement between the present results and that due to the results of Ref.[16] is excellent.

**Electron Number Density at Probe Locations**: Fig.11 and 12 show the electron number density obtained at the probe location which is situated at 1.2m axial distance from nose and is plotted along the wall normal direction. For the 61km altitude case, the near wall number density is about 4x10^{17}/m^3 and it reaches a peak of about 8x10^{17}/m^3. The flight predicted number density is of the same order as the present prediction. In comparison with the results of Ref.[16], the present data resembles the trend of VEENE data. For the 71km flight condition, near the wall, the electron number density is about 1.9x10^{17}/m^3 as compared to 1.0x10^{17}/m^3 due to VEENE data of Ref.[16]. It can be observed that, qualitatively, the prediction follows the trend of the electron non-equilibrium data of Ref.[16] and lie within the same order of magnitude of the flight data.

**Prediction of Blackout Frequency**: The plot of altitude versus flight speed during reentry [15] is shown in Fig.13. Also shown are the onset and end of blackout [15] of various antennae communication systems such as the VHF working at 259.7MHz, C-band working at 5.800MHz and X-band at 10.044MHz. The present simulation at altitudes of 61km and 71km fall within the communication blackout flight regime. Hence it is necessary to verify whether the predicted plasma frequency is of the same order when compared to the above mentioned antenna frequencies. This will prove the predictive capability of CERANS-TCNEQ for communication blackout studies. The plots of variation of plasma frequency obtained using equation (2) along the axial length of the body for both the flight altitude conditions are shown in Fig.14. For the 61km condition, the peak plasma frequency occurs at the nose which is about 30 GHz and it is about 16GHz for the 71km case. The plasma frequency decreases along the axial length and it reaches a value of 8GHz for the 61km case and about 5GHz case. Since the simulated plasma frequencies are comparable to the communication frequencies of the antennae, it is possible that the radio signals due to all the antennae shall get attenuated.

**Orbital Reentry Experiment Vehicle (OREX)**

**Geometry, Grid and Freestream Conditions**: The Orbital Reentry EXperiment [17] was conducted in 1994 jointly by National Aerospace Laboratory, Japan and the National Space Development Agency (NASA), Japan. During reentry of the OREX space vehicle, several useful measurements such as surface heat flux, surface pressure and electron number density were carried out at altitudes ranging from 105km to 48.4km. This experiment serves as a benchmark for comparing numerical computations with the flight data and for assessing and improving air-chemistry models.

The OREX geometry consists of a 50° sphere cone forebody followed by a tapered base. The nose radius of OREX body is 1350mm, overall length is 1508mm and the diameter is 3400mm. In the present study, only the forebody portion of the geometry is considered for simulations. The schematic of the OREX geometry is shown in Fig.15. The full details of the geometry and the electrostatic probe location are provided in Ref.[18]. Structured grid generated for the geometry is shown Fig.16. The grid size is 71x17x91 (71 points on the wall along axial length, 17 points along the circumference and 91 points away from the wall) amounting to about 100,000 hexahedral cells and is found to be optimal for this study. The near wall spacing of the first grid point is about 6x10^{-6}m. The table of freestream conditions [19] considered for simulations are shown in Table-5. The volumetric fractions of freestream atmospheric species considered for simulations...
are $N_2$ of 76.8% and $O_2$ of 23.2% corresponding to molar fractions of 79.1% of $N_2$ and 20.9% of $O_2$. For all these simulations, the flow is considered laminar and the wall is assumed as non catalytic.

It can be observed that within the flight duration considered for simulations, the flight altitude vary from about 84 km to about 48km and the freestream velocity vary from about 7.4km/sec to about 3.0km/sec.

<table>
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<th>Sl. No</th>
<th>Time 't' (sec)</th>
<th>Flight Time 't' (sec)</th>
<th>Altitude H (km)</th>
<th>Velocity $U_{\infty}$ (km/sec)</th>
<th>Temperature $T_{\infty}$ (K)</th>
<th>Pressure $P_{\infty}$ (N/m$^2$)</th>
<th>Wall Temperature (K)</th>
<th>Mach No. $M_{\infty}$</th>
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Description of Flow Features: Typical simulation results for the 84.01km altitude flight condition in the form of pressure contours are shown in Fig.17. The translational-rotational temperature and the vibrational temperature contours are shown in Fig.18 and 19 respectively. The pressure at stagnation point is predicted to be 567 N/m$^2$, which is about 955 times the freestream pressure. The shock standoff distance is about 0.107m ahead of the stagnation point. The post shock translational-rotational temperature is about 17,800K and the peak vibrational temperature is about 13,200K. Similar to the RAM-C II case, it can be observed that the gradient of translational-rotational temperature across the shock is much higher than the gradient of vibrational temperature.

Surface Pressure Distribution: The surface variation of pressure is presented in Fig.20. Due to the body curvature from the nose stagnation point and the resultant flow expansion, the surface pressure decreases from stagnation point value of 567N/m$^2$ to about 320N/m$^2$ at 1.0m distance from the stagnation point. Thereafter, due to the conical shape of the body, the flow undergoes a moderate compression and the pressure reaches a value of about 350N/m$^2$. At the aft end of the body, due to large curvature tending towards the base of the geometry, the flow expands sharply and the pressure drops to about 40N/m$^2$. The simulation results of Gupta [17], et al which is obtained with the Viscous Shock Layer (VSL) code is also plotted in Fig.20 for comparative purpose. It can be observed that the surface pressure variation due to the present result is in very good agreement with the VSL data.

Surface Heat Flux Distribution: The surface variation of heat flux depicted in Fig.21 shows that the stagnation point heat flux value is about 16 W/cm$^2$. The heat flux is maximum at the stagnation point and further decreases downstream before reaching a constant of about 9 W/cm$^2$ over the cone. Similar to the pressure variation, the heat flux reduces rapidly towards the aft end due to large body curvature on approaching the base. The heat flux distribution due to VSL results are also presented in Fig.21 and it can be observed that the CERANS-TCNEQ is able to mimic the trend though the stagnation heat flux due to VSL data is about 12 W/cm$^2$ which implies that the CERANS-TCNEQ data is higher than VSL data by about 33%. For the sake of completeness, the flight measured heat flux at stagnation point is also shown in Fig.21 which is about 14.5 W/cm$^2$ and the CERANS-TCNEQ data is higher than flight data by about 10%. Qualitatively, the results predicted by CERANS-TCNEQ are comparable to the results of these references.
**Electron Number Density at Probe Location**

The variation of electron number density at electrostatic probe locations is shown in Fig. 22. The electron number density at the wall is about \(1.0 \times 10^{18}/m^3\) and gradually decreases by about two-orders at probe location of 0.21m away from wall. The VSL data is plotted along with the CERANS-TCNEQ data and it can be observed that the present simulation is able to not only mimic the trend of number density variation, but has a very close agreement with the VSL data up to about 0.12m and beyond that the VSL data rapidly falls close to about three orders to \(1.0 \times 10^{15}/m^3\). When the present data and VSL data which have similar trends are plotted against the flight observed number density, a clear qualitative departure of the trend variation can be observed. The flight data shows a lower value of number density near to the wall of about 1.0 \times 10^{16}/m^3\) and increase away from the wall to \(2.0 \times 10^{18}/m^3\) for the available data up to 0.06m. The reason for discerning the difference in trends requires further in-depth analysis, such as possibility of including a three-temperature model with radiation effects and is beyond the scope of present work.

**Stagnation Point Heat Flux**

The variation of stagnation point heat flux at various flight conditions is plotted in Fig. 23. As the OREX configuration descends and reenters into the denser atmosphere, the stagnation point heat flux increases from about 16 W/cm\(^2\) at flight time of 7410 seconds to about 28 W/cm\(^2\) at about 7470 seconds and then decreases to about 10 W/cm\(^2\) at 7500 seconds. Comparison is drawn with the numerical simulation due to Doihara et al. which is a three-temperature non-catalytic wall based simulation and the flight data. The results of Doihara shows that the heat flux at 7410 seconds is about 13 W/cm\(^2\) and it reaches a peak value of about 31 W/cm\(^2\) at 7460 seconds. The trend of heat flux variation as depicted by the superimposed plots of these results show a good qualitative agreement. However, time variation of heat flux of flight data is steeper than the numerical solutions. Though the magnitude of heat flux is of the same order (14 W/cm\(^2\)) at 7410 seconds, the value corresponding to 7460 seconds where the peak occurs is about 41 W/cm\(^2\). It can be seen that the qualitative trend of a rise in heat flux from 7410 to 7460 seconds due to the numerical simulation is similar to that of the flight data and further followed by a decreasing trend after 7460 seconds except that here the slopes of the ascent and descent segment of heat flux is roughly half that of the flight data.

**Mole Fraction Distribution along the Stagnation Line**

The variation of mole fractions of all the seven species along the stagnation line distance normalized with the shock standoff distance, for flight conditions at 79.01km and 63.60 km altitude are shown in Figs. 24 and 25 respectively. The mole fractions are presented in logarithmic scale to highlight the enormous changes taking place in the post shock state. In both the cases, the variation of N2 species is shallow; however significant dissociation of N2 had taken place in the post shock state and the lowest N2 mole fraction is about 0.3 for the 79km case and about 0.4 for the 63km case. The mole fraction variation of O2 species clearly indicates that the values decrease by five orders of magnitude in the shock layer signifying the complete dissociation of the O2 molecules.

Due to large scale dissociation of N2 species into two N species, a significant amount of N species is formed and it almost remains constant after the shock. The peak value of N species mole fraction is about 0.39 for the 79 km case and it is about 0.33 for the 63km case. Due to complete dissociation of O2 into O species, a substantial amount of O species is present in post shock state till the stagnation point. The peak value of O mole fraction is about 0.26 for the 79km case and about 0.31 for the 63km case. Formation of NO species across the shock due to formation of N and O from the N2 and O2 dissociations is also significant and the peak value of NO mole fraction is about 0.009 for the 79km case and 0.042 for the 63 km case, occurring just behind the shock. However the mole fraction of NO species reduces by about 3 orders as the stagnation point is approached.

The NO+ and electron species are formed due to the dissociative recombination reaction and depends strongly on the formation of N and O species. The mole fraction variation of NO+ and e- species is the same as they originate as products of the only dissociative recombination reaction. Hence the number density of electrons and ions in the flow field will be the same and therefore their mole fractions are also the same. The peak mole fraction of the ion and electron species is of the order of \(10^{-3}\) for the 79km case and about \(7 \times 10^{-4}\) for the 63km case.

In order to qualitatively assess the performance of CERANS-TCNEQ for such a complex flow scenario, the present results are compared with the results obtained from Doihara et al. In both the cases, the mole fraction variation of all the species follow the same trend of Ref.[20] and the magnitude of spatial variation has a good agreement for the 79km case and an excellent agreement for the 63km case, despite being plotted in logarithmic scale. In case of the results of Doihara, the mole...
fraction of the NO+ and electron species differ due to formation of various other ionic species in the 11-species, three temperature model. Due to this the mole fraction variation of the ionic species due to CERANS-TCNEQ based on 7-species model can be marginally different from Ref.[20].

As an overall remark, the qualitative comparison of the present simulation results in terms of various flow parameters with that of Ref.[20] have been found to be quite close.

Conclusions and Further Work

A numerical simulation capability had been developed for modeling weakly ionized reentry flows. The two-temperature, 7-species, 18-reaction thermo-chemical non equilibrium, ionizing air-chemistry model of Park is implemented in a three dimensional finite volume solver called CERANS-TCNEQ. In the two-temperature model, the electron temperature equilibrates with the vibrational temperature and contribution of vibrational-electron-electronic energy of the reactive mixture is accounted in total energy equation as well as in the energy relaxation model. The energy transfer between translational and vibrational-electron-electronic energy modes had been modeled using the Landau-Teller relaxation model and the convective fluxes were modeled using the AUSM-PW+ numerical scheme. The code had been characterized for reentry flow case studies such as the RAM-C II as well as the OREX geometries. Comparison of various parameters such as the pressure distribution, heat flux distribution, mole fraction of various species and the two-temperatures along the stagnation line were found to be in good qualitative agreement with the available literature data. The electron number density predicted by CERANS-TCNEQ for all the test cases has good qualitative agreement with the results reported in open literature. The electron plasma frequency obtained from the present simulation for RAM-C II confirms the possible signal attenuation or blackout.

However further enhancements towards improving the predictive capability being considered as part of future work are (i) implementation of the 11 species air-chemistry model, (ii) implementation of Gupta’s collision-cross section based transport properties and (iii) inclusion of electronic non-equilibrium and the electronic-energy exchange mechanisms. In order for the code to be further useful for flow control studies such as aerobraking, introduction of magnetohydrodynamic (MHD) effects are being undertaken.

References


Fig. 3 Grid for RAM-C II

Fig. 4 Vibrational Temperature Contours (K)

Fig. 5 $T - T_v$ Distribution Along Stagnation Line (61 km Altitude)

Fig. 6 $T - T_v$ Distribution Along Stagnation Line (71 km Altitude)

Fig. 7 Peak Electron Number Density vs Axial Distance (61 km Altitude)
Fig. 8 Peak Electron Number Density vs Axial Distance (71 km Altitude)

Fig. 9 Electron Number Density Along Stagnation Line (61 km Altitude)

Fig. 10 Electron Number Density Along Stagnation Line (71 km Altitude)

Fig. 11 Electron Number at Probe Location (61 Altitude)
Fig. 12 Electron Number at Probe Location (71 km Altitude)

Fig. 13 Altitude-Velocity Plot Showing Communication Black Out [Ref. 15]

Fig. 14 Peak Plasma Frequency Along the Axial Length

Fig. 15 Geometry of OREX Configuration (mm)
Fig. 16 Grid for OREX Geometry

Fig. 17 Pressure Contours (N/m²)

Fig. 18 Temperature Contours, K

Fig. 19 T, Contours, K

Fig. 20 Pressure Distribution Over the Body (N/m²), 84.01 km Altitude

Fig. 21 Heat Flux Distribution Over the Body (W/cm²), 84.01 km Altitude
Fig. 22 Electron Number Density Along Probe Distance (l/m^3), 84.01 km Altitude

Fig. 23 Stagnation Heat Flux Along the Trajectory (W/cm^2)

Fig. 24 Mole Fraction Along Stagnation Line (79.01 km)

Fig. 25 Mole Fraction Along Stagnation Line (63.60 km)