Thermochemical Non-Equilibrium Reentry Flows in Three-Dimensions: Seven Species Model – Part I

Edisson S. G. Maciel, Amilcar P. Pimenta and Nikos E. Mastorakis

Abstract—This work presents a numerical tool implemented to simulate inviscid and viscous flows employing the reactive gas formulation of thermochemical non-equilibrium. The Euler and Navier-Stokes equations, employing a finite volume formulation, on the context of structured and unstructured spatial discretizations, are solved. These variants allow an effective comparison between the two types of spatial discretization aiming verify their potentialities: solution quality, convergence speed, computational cost, etc. The aerospace problem involving the hypersonic flow around a blunt body, in three-dimensions, is simulated. The reactive simulations will involve an air chemical model of seven species: N, O, N$_2$, O$_2$, NO, NO$^+$ and e. Eighteen chemical reactions, involving dissociation, recombination and ionization, will be simulated by the proposed model. This model was suggested by Blottner. The Arrhenius formula will be employed to determine the reaction rates and the law of mass action will be used to determine the source terms of each gas species equation. In this work is only presented the structured formulation and solutions. The unstructured formulation and solutions are presented in the second part of this study, which treats exclusively the unstructured context.

Keywords—Thermochemical non-equilibrium, Reentry flow, Seven species chemical model, Arrhenius formula, Structured and unstructured solutions, Euler and Navier-Stokes equations, Three-Dimensions.

I. INTRODUCTION

A HYPERSONIC flight vehicle has many applications for both military and civilian purposes including reentry vehicles such as the Space Shuttle and the Automated Transfer Vehicle (ATV) of the European Space Agency (ESA). The extreme environment of a hypersonic flow has a major impact on the design and analysis of the aerodynamic and thermal loading of a reentry or hypersonic cruise vehicle. During a hypersonic flight, the species of the flow field are vibrationally excited, dissociated, and ionized because of the very strong shock wave which is created around a vehicle. Because of these phenomena, it is necessary to consider the flow to be in thermal and chemical non-equilibrium.

In high speed flows, any adjustment of chemical composition or thermodynamic equilibrium to a change in local environment requires certain time. This is because the redistribution of chemical species and internal energies require certain number of molecular collisions, and hence a certain characteristic time. Chemical non-equilibrium occurs when the characteristic time for the chemical reactions to reach local equilibrium is of the same order as the characteristic time of the fluid flow. Similarly, thermal non-equilibrium occurs when the characteristic time for translation and various internal energy modes to reach local equilibrium is of the same order as the characteristic time of the fluid flow. Since chemical and thermal changes are the results of collisions between the constituent particles, non-equilibrium effects prevail in high-speed flows in low-density air.

In chemical non-equilibrium flows the mass conservation equation is applied to each of the constituent species in the gas mixture. Therefore, the overall mass conservation equation is replaced by as many species conservation equations as the number of chemical species considered. The assumption of thermal non-equilibrium introduces additional energy conservation equations – one for every additional energy mode. Thus, the number of governing equations for non-equilibrium flow is much bigger compared to those for perfect gas flow. A complete set of governing equations for non-equilibrium flow may be found in [1-2].

Analysis of non-equilibrium flow is rather complex because (1) the number of equations to be solved is much larger than the Navier-Stokes equations, and (2) there are additional terms like the species production, mass diffusion, and vibrational energy relaxation, etc., that appear in the governing equations. In a typical flight of the NASP (National AeroSpace Plane) flying at Mach 15, ionization is not expected to occur, and a 5-species air is adequate for the analysis (see [3]). Since the rotational characteristic temperatures for the constituent species (namely N, O, N$_2$, O$_2$ and NO) are small, the translational and rotational energy modes are assumed to be in equilibrium, whereas the
vibrational energy mode is assumed to be in non-equilibrium. 
[4] has simplified the thermodynamic model by assuming a
harmonic oscillator to describe the vibrational energy. Ionic
species and electrons are not considered. This simplifies the
set of governing equations by eliminating the equation
governing electron and electronic excitation energy. [4] has
taken the complete set of governing equations from [1], and
simplified them for a five-species two-temperature air model.

The problems of chemical non-equilibrium in the shock
layers over vehicles flying at high speeds and high altitudes in
the Earth’s atmosphere have been discussed by several
investigators ([5-8]). Most of the existing computer codes for
calculating the non-equilibrium reacting flow use the one-
temperature model, which assumes that all of the internal
energy modes of the gaseous species are in equilibrium with
the translational mode ([7-8]). It has been pointed out that such
a one-temperature description of the flow leads to a substantial
overestimation of the rate of equilibrium because of the
elevated vibrational temperature [6]. A three-temperature
chemical-kinetic model has been proposed by [9] to describe
the relaxation phenomena correctly in such a flight regime.
However, the model is quite complex and requires many
chemical rate parameters which are not yet known. As a
compromise between the three-temperature and the
conventional one-temperature model, a two-temperature
chemical-kinetic model has been developed ([10-11]), which is
designated herein as the TTv model. The TTv model uses one
temperature T to characterize both the translational energy of
the atoms and molecules and the rotational energy of the
molecules, and another temperature Tv to characterize the
vibrational energy of the molecules, translational energy of the
electrons, and electronic excitation energy of atoms and
molecules. The model has been applied to compute the
thermodynamic properties behind a normal shock wave in a
flow through a constant-area duct ([10-11]). Radiation
emission from the non-equilibrium flow has been calculated
using the Non-equilibrium Air Radiation (NEQAIR) program
([12-13]). The flow and the radiation computations have been
packaged into a single computer program, the Shock-Tube
Radiation Program (STRAP) ([11]).

A first-step assessment of the TTv model was made in [11]
where it was used in computing the fAlow properties and
radiation emission from the flow in a shock tube for pure
nitrogen undergoing dissociation and weak ionization
(ionization fraction less than 0.1%). Generally good agreement
was found between the calculated radiation emission and those
obtained experimentally in shock tubes ([14-16]). The only
exception involved the vibrational temperature. The theoretical
treatment of the vibrational temperature could not be validated
because the existing data on the vibrational temperature behind
a normal shock wave ([16]) are those for an electronically
excited state of the molecular nitrogen ion N2+ instead of the
ground electronic state of the neutral nitrogen molecule N2
which is calculated in the theoretical model. The measured
vibrational temperature of N2+ was much smaller than the
calculated vibrational temperature for N2.

This work, first of this study, describes a numerical tool to
perform thermochemical non-equilibrium simulations of
reactive flow in three-dimensions. The [17] scheme, in its first-
and second-order versions, is implemented to accomplish the
numerical simulations. The Euler and Navier-Stokes equations,
on a finite volume context and employing structured and
unstructured spatial discretizations, are applied to solve the
“hot gas” hypersonic flow around a blunt body in two-
dimensions. The second-order version of the [17] scheme is
obtained from a “MUSCL” extrapolation procedure in a
context of structured spatial discretization. In the unstructured
context, only first-order solutions are obtained. The
convergence process is accelerated to the steady state
condition through a spatially variable time step procedure,
which has proved effective gains in terms of computational
acceleration (see [18-19]). In this paper only the structured
formulation and results are presented.

The reactive simulations involve an air chemical model of
seven species: N, O, N2, O2, NO, NO+ and e+. Eighteen
chemical reactions, involving dissociation, recombination and
ionization, are simulated by the proposed model. This model
was suggested by [46]. The Arrhenius formula is employed to
determine the reaction rates and the law of mass action is used
to determine the source terms of each gas species equation.

The results have demonstrated that the shock position is
closer to the geometry as using the reactive formulation, the
stagnation pressure is better estimated by the [17] scheme, in
its first-order, viscous, structured formulation, and the standoff
distance is better predicted by its second-order, viscous,
structured formulation.

II. FORMULATION TO REACTIVE FLOW IN THERMOCHEMICAL
NON-EQUILIBRIUM

A. Reactive Equations in Three-Dimensions

The reactive Navier-Stokes equations in thermal and chemical
non-equilibrium were implemented on a finite volume context,
in the three-dimensional space. In this case, these equations in
integral and conservative forms can be expressed by:

\[
\frac{\partial}{\partial t} \int_{V} Q dV + \int_{S} \mathbf{F} \cdot \mathbf{n} dS = \int_{S_{CV}} dV , \quad \text{with}
\]

\[
\mathbf{F} = (E_e - E_v) \mathbf{i} + (F_e - F_v) \mathbf{j} + (G_e - G_v) \mathbf{k} ,
\]

where: Q is the vector of conserved variables, V is the volume
of a computational cell, F is the complete flux vector, n is the
unity vector normal to the flux face, S is the flux area, S_{CV} is
the chemical and vibrational source term, E_e, F_e, and G_e are
the convective flux vectors or the Euler flux vectors in the x, y and
z directions, respectively. E_v, F_v, and G_v are the viscous flux
vectors in the x, y and z directions, respectively. The \( \mathbf{i}, \mathbf{j} \) and \( \mathbf{k} \) unity vectors define the Cartesian coordinate system.

Twelve (12) conservation equations are solved: one of general
mass conservation, three of linear momentum conservation,
one of total energy, six of species mass conservation and one of
the vibrational internal energy of the molecules. Therefore,
one of the species is absent of the iterative process. The CFD
(“Computational Fluid Dynamics”) literature recommends that the species of biggest mass fraction of the gaseous mixture should be omitted, aiming to result in a minor numerical accumulation error, corresponding to the biggest mixture constituent (in the case, the air). To the present study, in which is chosen a chemical model to the air composed of seven (7) chemical species (N, O, N₂, O₂, NO, NO⁺ and e⁻) and eighteen (18) chemical reactions, being fifteen (15) dissociation reactions (endothermic reactions), two (2) of exchange or recombination, and one (1) of ionization, this species can be either the N₂ or the O₂. To this work, it was chosen the N₂. The vectors Q, Eₓ, Eᵧ, Gₓ, Eᵥ, Fₓ, Gᵧ, and Sᵥᵥ can, hence, be defined as follows ([4]):

\[
Q = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
e \\
\rho_1 u \\
\rho_2 u \\
\rho_3 u \\
\rho_4 u \\
\rho_5 u \\
\rho_6 u \\
\rho_7 u \\
\rho e_y \\
\rho e_y u
\end{bmatrix}, \quad E_x = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho v u \\
\rho v w \\
e u \\
\rho_1 u^2 \\
\rho_2 u^2 \\
\rho_3 u^2 \\
\rho_4 u^2 \\
\rho_5 u^2 \\
\rho_6 u^2 \\
\rho_7 u^2 \\
\rho e_y u \\
\rho e_y u^2
\end{bmatrix}, \quad F_x = \begin{bmatrix}
\rho v \\
\rho v u \\
\rho v^2 + p \\
\rho w v \\
e v \\
\rho_1 v \\
\rho_2 v \\
\rho_3 v \\
\rho_4 v \\
\rho_5 v \\
\rho_6 v \\
\rho_7 v \\
\rho e_y v \\
\rho e_y v^2
\end{bmatrix}, \quad G_x = \begin{bmatrix}
\rho w \\
\rho w u \\
\rho w v \\
\rho w^2 + p \\
e w \\
\rho_1 w \\
\rho_2 w \\
\rho_3 w \\
\rho_4 w \\
\rho_5 w \\
\rho_6 w \\
\rho_7 w \\
\rho e_y w \\
\rho e_y w^2
\end{bmatrix}; (2)
\]

\[
E_y = \frac{1}{Re} \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
\tau_{xy} u + \tau_{xy} v + \tau_{xz} w - q_{f,x} - \phi_x - \phi_{v,x} \\
-\rho_1 v_{1x} \\
-\rho_2 v_{2x} \\
-\rho_3 v_{4x} \\
-\rho_5 v_{5x} \\
-\rho_6 v_{6x} \\
-\rho_7 v_{7x} \\
-q_{v,x} - \phi_{v,x}
\end{bmatrix}, (3a)
\]

\[
G_y = \frac{1}{Re} \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
\tau_{xy} u + \tau_{xy} v + \tau_{xz} w - q_{f,x} - q_{v,x} - \phi_{v,x} \\
-\rho_1 v_{1x} \\
-\rho_2 v_{2x} \\
-\rho_3 v_{4x} \\
-\rho_5 v_{5x} \\
-\rho_6 v_{6x} \\
-\rho_7 v_{7x} \\
-q_{v,x} - \phi_{v,x}
\end{bmatrix}; (3c)
\]

\[
S_{v,v} = \sum_{s=\text{mol}} \rho_s \left( e_{v,s}^* - e_{v,s} \right) / \tau_s + \sum_{s=\text{mol}} \phi_s e_{v,s}, (4)
\]

in which: \( \rho \) is the mixture density; \( u, v \) and \( w \) are Cartesian components of the velocity vector in the \( x, y \) and \( z \) directions, respectively; \( p \) is the fluid static pressure; \( e \) is the fluid total energy; \( \rho_1, \rho_2, \rho_4, \rho_5, \rho_6, \rho_7 \) are densities of the N, O, O₂, NO, NO⁺ and e⁻, respectively; \( H \) is the mixture total enthalpy; \( e \), is the sum of the vibrational energy of the molecules; the \( \tau \)'s are the components of the viscous stress tensor; \( q_{f,x}, q_{f,y} \) and \( q_{f,z} \) are the frozen components of the Fourier-heat-flux vector in the \( x, y \) and \( z \) directions, respectively; \( q_{v,x}, q_{v,y} \) and \( q_{v,z} \) are the components of the Fourier-heat-flux vector calculated with the vibrational thermal conductivity and vibrational temperature; \( \rho_v v_x, \rho_v v_y \) and \( \rho_v v_z \) represent the species diffusion flux, defined by the Fick law; \( \phi_x, \phi_y \) and \( \phi_z \) are the terms of mixture diffusion; \( \phi_{v,x}, \phi_{v,y} \) and \( \phi_{v,z} \) are the terms of molecular diffusion calculated at the vibrational temperature; \( \phi \) is the chemical source term of each species equation, defined by the law of mass action; \( e_v \) is the molecular-vibrational-internal energy calculated with the translational/rotational temperature; and \( \tau \) is the translational-vibrational characteristic relaxation time of each molecule.
The viscous stresses, in N/m², are determined, according to a Newtonian fluid model, by:

\[
\begin{align*}
\tau_{xx} &= 2\mu \frac{\partial u}{\partial x} - 2 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \\
\tau_{yy} &= 2\mu \frac{\partial v}{\partial y} - 2 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \\
\tau_{zz} &= 2\mu \frac{\partial w}{\partial z} - 2 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \\
\tau_{xy} &= \tau_{yx} = \mu \left( \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right), \\
\tau_{xz} &= \tau_{zx} = \mu \left( \frac{\partial v}{\partial z} - \frac{\partial w}{\partial y} \right), \\
\tau_{yz} &= \tau_{zy} = \mu \left( \frac{\partial w}{\partial x} - \frac{\partial v}{\partial z} \right),
\end{align*}
\] (5)

in which \(\mu\) is the fluid molecular viscosity.

The frozen components of the Fourier-heat-flux vector, which considers only thermal conduction, are defined by:

\[
q_{f,x} = -k_f \frac{\partial T}{\partial x}, \quad q_{f,y} = -k_f \frac{\partial T}{\partial y}, \quad q_{f,z} = -k_f \frac{\partial T}{\partial z},
\] (7)

where \(k_f\) is the mixture frozen thermal conductivity. The vibrational components of the Fourier-heat-flux vector are calculated as follows:

\[
q_{v,x} = -k_v \frac{\partial T}{\partial x}, \quad q_{v,y} = -k_v \frac{\partial T}{\partial y}, \quad q_{v,z} = -k_v \frac{\partial T}{\partial z},
\] (8)

in which \(k_v\) is the vibrational thermal conductivity and \(T_v\) is the vibrational temperature, what characterizes this model as of two temperatures: translational/rotational and vibrational.

The terms of species diffusion, defined by the Fick law, to a condition of thermal non-equilibrium, are determined by ([4]):

\[
\rho_s v_{sx} = -D_s \frac{\partial Y_{MF,s}}{\partial x}, \quad \rho_s v_{sy} = -D_s \frac{\partial Y_{MF,s}}{\partial y};
\] (9)

\[
\rho_s v_{sz} = -D_s \frac{\partial Y_{MF,s}}{\partial z},
\]

with “s” refer to a given species, \(Y_{MF,s}\) being the molar fraction of the species, defined as:

\[
Y_{MF,s} = \frac{\rho_s / M_s}{\sum_{k=1}^{ns} \rho_k / M_k}
\] (10)

and \(D_s\) is the species-effective-diffusion coefficient.

The diffusion terms \(\phi_x, \phi_y\) and \(\phi_z\) which appear in the energy equation are defined by ([20]):

\[
\phi_x = \sum_{s=1}^{ns} \rho_s \nu_{sx} h_s, \quad \phi_y = \sum_{s=1}^{ns} \rho_s \nu_{sy} h_s, \quad \phi_z = \sum_{s=1}^{ns} \rho_s \nu_{sz} h_s,
\] (11)

being \(h_s\) the specific enthalpy (sensible) of the chemical species “s”. Details of the calculation of the specific enthalpy, see [21-22]. The molecular diffusion terms calculated at the vibrational temperature, \(\phi_{v,x}, \phi_{v,y}\) and \(\phi_{v,z}\) which appear in the vibrational-inner-internal-energy equation are defined by ([4]):

\[
\phi_{v,x} = \sum_{s=\text{mol}}^{\text{mol}} \rho_s \nu_{sx} h_{v,s}, \quad \phi_{v,y} = \sum_{s=\text{mol}}^{\text{mol}} \rho_s \nu_{sy} h_{v,s}; \quad \phi_{v,z} = \sum_{s=\text{mol}}^{\text{mol}} \rho_s \nu_{sz} h_{v,s},
\] (12)

with \(h_{v,s}\) being the specific enthalpy (sensible) of the chemical species “s” calculated at the vibrational temperature \(T_v\). The sum of Eq. (12), as also those present in Eq. (5), considers only the molecules of the system, namely: N₂, O₂, NO, and NO⁺.

B. Thermodynamic Model/Thermodynamic Properties

Definition of general parameters.

\[
p = RT \sum_{s=1}^{ns} \rho_s / M_s = p \sigma RT, \quad \sigma = \sum_{s=1}^{ns} \rho_s / M_s = \sum_{s=1}^{ns} c_s / M_s \Rightarrow \sigma = \sum_{s=1}^{ns} c_s / M_s,
\] (13)

in which: \(\sigma\) is the mixture number in kg-mol/kg and \(c_s\) is the mass fraction (non-dimensional), defined by \(c_s = \rho_s / p\).

\[
\sigma = \sum_{s=1}^{ns} \sigma_s \Rightarrow \sigma_s = c_s / M_s;
\]

\[
M_{\text{mixt}} = 1 / \sigma \Rightarrow M_{\text{mixt}} = \frac{1}{\sum_{s=1}^{ns} c_s / M_s};
\]

\[
e_{v,s}^* = e_{v,s} (T_v = T),
\] (14)

with: \(\sigma_s\) being the number of kg-mol/kg of species “s” and \(M_{\text{mixt}}\) is the mixture molecular mass, in kg/kg-mol.

Thermodynamic model.

(a) Mixture translational internal energy:

\[
e_T = \sum_{s=1}^{ns} e_{T,s} \sigma_s = \sum_{s=1}^{ns} \left[ \int_0^T C_{v,T,s}(T) dT + h^0 \right] \sigma_s,
\] (15)

where: \(e_{T,s}\) is the translational internal energy per kg-mol of species “s”, in J/kg-mol. The specific heat at constant volume per kg-mol of species “s” due to translation, in J/(kg-mol·K), is
defined by:

\[ C_{v,T,s}(T) = 1.5R. \]  

(16)

Hence,

\[ e_{T,s}(T) = 1.5RT + h_0^0 \Rightarrow e_{T}(T) = \sum_{s=1}^{m_s} \sigma_s \left[ 1.5RT + h_0^0 \right], \]  

(17)

with: \( e_T \) being the translational internal energy per unity of the gaseous mixture mass, in J/kg, and \( h_0 \) being the formation enthalpy of the species “s” per kg-mol of species, J/kg-mol. It is important to note that:

\[ e_T(T) = \sum_{s=1}^{m_s} \sigma_s \left[ 1.5RT + h_0^0 \right] = \sum_{s=1}^{m_s} c_s \left[ 1.5RT + h_0^0 \right], \]  

(18)

with: \( R_s \) being the gas constant of species “s” and \( h_0^0 \) being the formation enthalpy of species “s” in J/kg. The species formation enthalpy per g-mol of species is specified in Tab. 1.

Table 1 Species formation enthalpy.

<table>
<thead>
<tr>
<th>Species</th>
<th>( h_0 ) (J/g-mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>470,816.0</td>
</tr>
<tr>
<td>O</td>
<td>246,783.0</td>
</tr>
<tr>
<td>N(_2)</td>
<td>0.0</td>
</tr>
<tr>
<td>O(_2)</td>
<td>0.0</td>
</tr>
<tr>
<td>NO</td>
<td>90,671.0</td>
</tr>
<tr>
<td>NO(^*)</td>
<td>992,963.2</td>
</tr>
<tr>
<td>e(^*)</td>
<td>0.0</td>
</tr>
</tbody>
</table>

As can be noted, dividing each above term by the species molecular mass and multiplying by \( 10^3 \), it is possible to obtain the formation enthalpy in J/kg.

(b) Mixture rotational internal energy:

\[ e_R = \sum_{s=1}^{m_s} e_{R,s} \sigma_s = \sum_{s=1}^{m_s} \left[ \int_0^{T_s} C_{v,R,s}(T) dT \right] \sigma_s = \sum_{s=1}^{m_s} \sigma_s \int_0^T C_{v,R,s}(T) dT', \]  

(19)

where: \( e_{R,s} \) is the rotational internal energy per kg-mol of species “s”, in J/kg-mol. The specific heat at constant volume per kg-mol of species “s” due to rotation, in J/(kg-mol-K), is defined by:

\[ C_{v,R,s} = R \Rightarrow e_{R,s}(T) = RT \Leftrightarrow e_{R}(T) = \sum_{s=1}^{m_s} C_{v,R,s}RT \]

or

\[ e_R(T) = \sum_{s=1}^{m_s} c_s R_s T. \]  

(20)

with \( e_R \) being the rotational internal energy per unity of gaseous mixture mass, in J/kg.

(c) Mixture vibrational internal energy:

\[ e_v = \sum_{s=1}^{m_s} e_{v,s} \sigma_s = \sum_{s=1}^{m_s} \left[ \int_0^{T_s} C_{v,V,s}(T) dT \right] \sigma_s = \sum_{s=1}^{m_s} \sigma_s \int_0^T C_{v,V,s}(T) dT'. \]  

(21)

in which: \( e_v \) is the vibrational internal energy per unity of gaseous mixture mass, in J/kg; \( e_{v,s} \) is the vibrational internal energy per kg-mol of species “s”, in J/kg-mol; \( C_{v,V,s} \) is the specific heat at constant volume per kg-mol of species “s” due to vibration, in J/(kg-mol-K); \( \theta_{v,s} \) is the characteristic vibrational+ temperature of species “s”, in K; and \( T_s \) is the vibrational temperature, in K. The characteristic vibrational temperature to each molecule is specified in Tab. 2, obtained from [4]. It is important to note that \( e_v \) is also directly obtained from the vector of conserved variables.

Table 2 Characteristic vibrational temperature of the molecular species.

<table>
<thead>
<tr>
<th>Species</th>
<th>N(_2)</th>
<th>O(_2)</th>
<th>NO</th>
<th>NO(^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_{v,s} ) (K)</td>
<td>3,390.0</td>
<td>2,270.0</td>
<td>2,740.0</td>
<td>2,740.0</td>
</tr>
</tbody>
</table>

It is important to note that the modes of translational and rotational internal energy are assumed completely excited and, hence, the specific heats at constant volume to these modes are temperature independent. The vibrational-internal-energy mode is admitted not be completely excited, and, hence, the vibrational specific heat at constant volume is function of the vibrational temperature. The expression above to \( C_{v,V,s} \) is due to [23] and is the result of the hypothesis that the molecules can be considered as harmonic oscillators. Note that when the mode of vibrational internal energy is completely excited, i.e., when \( T_s \gg \theta_{v,s} \), \( C_{v,V,s} = R \).

(c) Mixture internal energy:

\[ e_{int} = e_T + e_R + e_v. \]  

(22)

which is the internal energy per unity of mixture mass, in J/kg.

(d) Frozen speed of sound:

\[ C_{v,TR} = \sum_{s=1}^{m_s} \sigma_s C_{v,TR,s} = \sum_{s=1}^{m_s} \left( 2.5R \right) \text{ molecules per kg-mol}. \]  

\[ \beta = R\sigma/C_{v,TR} \cdot \sqrt{(\beta + 1)p/\rho}. \]  

(23)

The frozen speed of sound, in a thermochemical non-equilibrium model, should be employed in the calculation of the convective flux of the [17] scheme. \( C_{v,TR,s} \) is the specific heat at constant volume due to translation and rotation; in other words, \( C_{v,TR,s} \) is the sum of \( C_{v,T,s} \) with \( C_{v,R,s} \).
(e) Determination of the translational/rotational temperature:
\[
e = \sum_{s=1}^{m} c_s C_{v,TR,s} T + \sum_{s=1}^{m} c_s h_s^0 - e_V + \frac{1}{2} (u^2 + v^2 + w^2),
\]
(24)
to the three-dimensional case. Hence, noting that T is constant at the right hand side of Eq. (24), it is possible to write:
\[
T = \frac{1}{\sum_{s=1}^{m} c_s C_{v,TR,s}} \left[ e - \sum_{s=1}^{m} c_s h_s^0 - e_V - \frac{1}{2} (u^2 + v^2 + w^2) \right],
\]
(25)
to the three-dimensional case;

(f) Determination of the vibrational temperature:

The vibrational temperature is calculated through an interactive process employing the Newton-Raphson method (a version to the five species model is found in [24]).

(g) Species pressure:

Applying the equation of a thermally perfect gas to each species:
\[
p_s = \rho_s R_s T,
\]
(26)
where: \(\rho_s = c_s \rho\) is the density of species “s”, \(R_s\) is the gas constant to species “s” and T is the translational/rotational temperature.

C. Transport Model/Transport Physical Properties

**Collision integrals to species i and j.** In Table 3 are presented values of \(\log_{10} [\pi \Omega_{i,j}^{(1,1)}]\) and \(\log_{10} [\pi \Omega_{i,j}^{(2,2)}]\) to temperature values of 2,000 K and 4,000 K. The indexes i and j indicate, in the present case, the collision partners; in other words, the pair formed by one atom and one atom, one atom and one molecule, etc. These data obtained from [1].

The data aforementioned define a linear interpolation to values of \(\log_{10} [\pi \Omega_{i,j}^{(k,k)}]\) as function of Ln(T), with \(k = 1, 2\), through the linear equation:
\[
\log_{10} [\pi \Omega_{i,j}^{(k,k)}] (T) = \log_{10} [\pi \Omega_{i,j}^{(k,k)}] (T = 2,000 K) + \text{slope} \times \text{Ln}(T/2,000),
\]
(27)
in which:
\[
\text{slope} = \left( \frac{\log_{10} [\pi \Omega_{i,j}^{(k,k)}] (T = 4,000 K) - \log_{10} [\pi \Omega_{i,j}^{(k,k)}] (T = 2,000 K)}{\text{Ln} 2} \right).
\]
(28)
The value of \(\pi \Omega_{i,j}^{(k,k)}\) is obtained from:

\[
\pi \Omega_{i,j}^{(k,k)}(T) = e^{\left( \log_{10} [\pi \Omega_{i,j}^{(k,k)}] (T = 2,000 K) + \text{slope} \times \text{Ln}(T/2,000) \right)}.
\]
(29)
\[
\text{with the value of } \Omega_{i,j}^{(k,k)} \text{ in m}^3.
\]

<table>
<thead>
<tr>
<th>Pairs</th>
<th>(\log_{10} [\pi \Omega_{i,j}^{(1,1)}])</th>
<th>(\log_{10} [\pi \Omega_{i,j}^{(2,2)}])</th>
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</tbody>
</table>
Table 3 Collision integrals to five chemical species: N, O, N2, O2, NO, NO+ and e-. (Continuation)

<table>
<thead>
<tr>
<th>Pairs</th>
<th>Log_{10}[\pi \Omega_{i,j}^{(1,1)}]</th>
<th>Log_{10}[\pi \Omega_{i,j}^{(2,2)}]</th>
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<td>i</td>
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<tr>
<td>e'</td>
<td>O</td>
<td>-15.94</td>
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<tr>
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<td>N2</td>
<td>-15.11</td>
</tr>
<tr>
<td>e'</td>
<td>NO</td>
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<td>NO+</td>
<td>-11.70</td>
</tr>
<tr>
<td>e'</td>
<td>e'</td>
<td>-11.70</td>
</tr>
</tbody>
</table>

Modified collision integrals to the species i and j. [1] and [4] define the modified collision integrals to the species i and j as:

\[ \Delta_{i,j}^{(1)}(T) = \frac{8}{3} \sqrt{\frac{2m_{i,j}}{\pi RT}} \Omega_{i,j}^{(1,1)} \]  
\[ \Delta_{i,j}^{(2)}(T) = \frac{16}{5} \sqrt{\frac{2m_{i,j}}{\pi RT}} \Omega_{i,j}^{(2,2)}, \]  

(30)

with:

\[ m_{i,j} = M_i M_j / (M_i + M_j), \]  

(31)

being the reduced molecular mass. These integrals are given in m.s. With the definition of the modified collision integrals to species i and j, it is possible to define the mixture transport properties (viscosity and thermal conductivities) and the species diffusion property (diffusion coefficient).

Mixture molecular viscosity. [4] define the mixture molecular viscosity as:

\[ \mu_{\text{mix}} = \sum_{i=1}^{ns} \sum_{j=1}^{ns} m_i \sigma_i \Delta_{i,j}^{(2)}(T), \]  

(32)

where:

\[ m_i = M_i / N_{\text{AV}}, \]  

(33)

being the mass of a species particle under study. \( N_{\text{AV}} = 6.022045 \times 10^{23} \) particles/g-mol, Avogadro number. This mixture molecular viscosity is given in kg/(m.s).

Vibrational, frozen, rotational and translational thermal conductivities. All thermal conductivities are expressed in J/(m.s.K). [4] defines the mixture vibrational, rotational and translational thermal conductivities, as also the species diffusion coefficient, as follows.

(a) Translational thermal conductivity:
The mode of translational internal energy is admitted completely excited; hence, the thermal conductivity of the translational internal energy is determined by:

\[ k_T = \frac{15}{4} k_{\text{Boltzmann}} \sum_{i=1}^{ns} \frac{\sigma_i}{\sum_{j=1}^{ns} \tilde{a}_{i,j} \Delta_{i,j}^{(2)}(T)}, \]  

(34)

in which:

\[ k_{\text{Boltzmann}} = \text{Boltzmann constant} = 1.380622 \times 10^{-23} J/K; \]
\[ \tilde{a}_{i,j} = 1 + \frac{(1 - M_i / M_j)0.45 - 2.54[M_i / M_j]}{[1 + M_i / M_j]^2}. \]  

(35)

(b) Rotational thermal conductivity:
The mode of rotational internal energy is also considered fully excited; hence, the thermal conductivity due to rotational internal energy is defined by:

\[ k_R = k_{\text{Boltzmann}} \sum_{i=1}^{ns} \sum_{j=1}^{ns} \sigma_i \Delta_{i,j}^{(3)}(T). \]  

(36)

(c) Frozen thermal conductivity:

\[ k_f = k_T + k_R. \]  

(37)

(d) Thermal conductivity due to molecular vibration:
The mode of vibrational internal energy, however, is assumed to be partially excited; hence, the vibrational thermal conductivity is calculated according to [3] by:

\[ k_V = k_{\text{Boltzmann}} \sum_{i=1}^{ns} \frac{C_{i,V \alpha}}{R} \sigma_i \]  

(38)

with \( C_{i,V \alpha} \) obtained from Eq. (21).

Species diffusion coefficient. The mass-diffusion-effective coefficient, \( D_i \), of the species “i” in the gaseous mixture is defined by:

\[ D_i = \frac{\sigma_i^2 M_i (1 - \sigma_i M_i)}{\sum_{j=1}^{ns} \sigma_j / D_{i,j}} \]  

(39)

where: \( D_{i,j} \) is the binary diffusion coefficient to a pair of particles of the species “i” and “j” and is related with the modified collision integral conform described above, in Eq. (39). This coefficient is measured in m2/s.

D. Chemical Model
The chemical model employed to this case of thermochemical non-equilibrium is the seven species model of [46], using the
N, O, N₂, O₂, NO, NO⁺ and e⁻ species. This formulation uses, in the calculation of the species production rates, a temperature of reaction rate control, introduced in the place of the translational/rotational temperature, which is employed in the calculation of such rates. This procedure aims a couple between vibration and dissociation. This temperature is defined as: \( T_{\text{trc}} = \sqrt{T \times T_v} \), where \( T \) is the translational/rotational temperature and \( T_v \) is the vibrational temperature. This temperature \( T_{\text{trc}} \) replaces the translational/rotational temperature in the calculation of the species production rates, according to [25].

**Law of Mass Action.** The symbolic representation of a given reaction in the present work follows the [26] formulation and is represented by:

\[
\sum_{s=1}^{ns} v_{sr} A_s \leftrightarrow \sum_{r=1}^{ns} v_{sr} A_s, \quad r = 1, \ldots, nr. \tag{40}
\]

The law of mass action applied to this system of chemical reactions is defined by:

\[
\dot{\chi}_s = M \sum_{r=1}^{nr} \left( v_{sr} - v_{sr}' \right) k_f \prod_{s=1}^{ns} \left( \frac{\rho_s}{M_s} \right)^{v_{sr}} - k_{br} \prod_{s=1}^{ns} \left( \frac{\rho_s}{M_s} \right)^{v_{sr}'}, \tag{41}
\]

where \( A_s \) represents the chemical symbol of species “s”, “ns” is the number of species of the present study (reactants and products) involved in the considered reaction; “nr” is the number of reactions considered in the chemical model; \( v_{sr} \) e \( v_{sr}' \) are the stoichiometric coefficients to reactants and products, respectively; \( k_f = AT^B \mathrm{e}^{-C/T} \) and \( k_{br} = DT^E \), with A, B, C, D and E being constants of a specific chemical reaction under study [“fr” = forward reaction and “br” = backward reaction].

**Table 4. Chemical reactions and forward coefficients.**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward reaction rate coefficients, kfr, cm³/(mol·s)</th>
<th>Third body</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O}_2+\text{M} \leftrightarrow \text{2O}+\text{M} )</td>
<td>3.61x1018T-1.0e(-59,400/T)</td>
<td>O, N, O₂, N₂, NO</td>
</tr>
<tr>
<td>( \text{N}_2+\text{M} \leftrightarrow \text{2N}+\text{M} )</td>
<td>1.92x1017T-0.5e(-113,100/T)</td>
<td>O, O₂, N₂, NO</td>
</tr>
<tr>
<td>( \text{N}_2+\text{N} \leftrightarrow \text{2N}+\text{N} )</td>
<td>4.52x1022T-0.5e(-113,100/T)</td>
<td>-</td>
</tr>
<tr>
<td>( \text{NO}+\text{M} \leftrightarrow \text{N}+\text{O}+\text{M} )</td>
<td>3.97x1020T-1.5e(-75,600/T)</td>
<td>O, O₂, N₂, NO</td>
</tr>
<tr>
<td>( \text{NO}+\text{O} \leftrightarrow \text{O}_2+\text{N} )</td>
<td>3.18x1097T1.0e(-19,700/T)</td>
<td>-</td>
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<tr>
<td>( \text{N}_2+\text{O} \leftrightarrow \text{NO}+\text{N} )</td>
<td>6.75x1013e(-37,500/T)</td>
<td>-</td>
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<tr>
<td>( \text{N}+\text{O} \leftrightarrow \text{NO}+\text{e}^- )</td>
<td>9.03x109e(-32,400/T)</td>
<td>-</td>
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</tbody>
</table>

It is important to note that \( k_{sr} = k_f / k_{sr}' \), with ker being the equilibrium constant which depends only of the thermodynamic quantities. In this work, \( ns = 7 \) and \( nr = 18 \). Table 4 presents the values to A, B, C, D and E for the forward reaction rates of the 18 chemical reactions. Table 5 presents the values to A, B, C, D and E for the backward reaction rates.

The eighth equation takes into account the formation of an electron from the ionization of the NO. For this case, the backward reaction rate depends only of the vibrational temperature.

**E. Vibrational Model**

The vibrational internal energy of a molecule, in J/kg, is defined by:

\[
e_{v,s} = \frac{R_s \theta_{v,s}}{e^{\theta_{v,s}/T_{v,s}} - 1}, \tag{42}
\]

obtained by the integration of Eq. (21), and the vibrational internal energy of all molecules is given by:

\[
e_V = \sum_{s=1}^{mol} e_{v,s} \cdot \tag{43}
\]

The heat flux due to translational-vibrational relaxation, according to [27], is given by:

\[
q_{T-V,s} = \rho_s \frac{e_{v,s}^* (T) - e_{v,s} (T_{v,s})}{\tau_s}, \tag{44}
\]

where \( e_{v,s}^* \) is the vibrational internal energy calculated at the translational temperature to the species “s”; and \( \tau_s \) is the translational-vibrational relaxation time to the molecular species, in s. The relaxation time is the time of energy exchange between the translational and vibrational molecular modes.
**Vibrational characteristic time of [28].** According to [28], the relaxation time of molar average of [29] is described by:

\[ \tau_s = \tau_{s,M-W} = \sum_{i=1}^{m_s} X_i / \tau_{s,M-W}, \]  

(45)

with:

\[ \tau_{s,M-W}^{i} \]  

is the relaxation time between species of [29];

\[ \tau_{s,M-W}^{s} \]  

is the vibrational characteristic time of [29];

\[ X_i = c_i / (N_{AV} m_i) \]  

and \( m_i = M_i / N_{AV} \).  

(46)

**Definition of \( \tau_{s,M-W} \).** For temperatures inferior to or equal to 8,000 K, [29] give the following semi-empirical correlation to the vibrational relaxation time due to inelastic collisions:

\[ \tau_{s,M-W}^{s,l} = \left( \frac{B}{p_1} \right) e^{[A_{s,l}(T^{-0.015}l_{ij}^{-0.4})-18.42]}, \]  

(47)

where:

\[ B = 1.013 \times 10^5 \text{Ns/m}^2 \]  

([30]);

\[ p_1 \]  

is the partial pressure of species “l” in N/m²;

\[ A_{s,l} = 1.16 \times 10^{-3} \mu_{s,l}^{1/2} T^{3/4} \]  

([30]);

\[ \mu_{s,l} = \frac{M_s M_l}{M_s + M_l}, \]  

(48)

being the reduced molecular mass of the collision partners: kg/kg-mol;

\( T \) and \( \theta_{s,a} \) in Kelvin.

**Correction time.** For temperatures superior to 8,000 K, the Eq. (43) gives relaxation times less than those observed in experiments. To temperatures above 8,000 K, [25] suggests the following relation to the vibrational relaxation time:

\[ \tau_{s}^p = \frac{1}{\xi_s \sigma v n_s}, \]  

(50)

where:

\[ \xi_s = \sqrt{\frac{8R}{\pi} T}, \]  

(51)

being the molecular average velocity in m/s;

\[ \sigma_v = 10^{-20} \left( \frac{50,000}{T} \right)^2, \]  

(52)

being the effective collision cross-section to vibrational relaxation in m²; and

\[ n_s = \rho_s / m_s, \]  

(53)

being the density of the number of collision particles of species “s”. \( \rho_s \) in kg/m³ and \( m_s \) in kg/particle, defined by Eq. (33).

Combining the two relations, the following expression to the vibrational relaxation time is obtained:

\[ \tau_s = \tau_{s,M-W}^p + \tau_s^p. \]  

(54)

[25] emphasizes that this expression [Eq. (54)] to the vibrational relaxation time is applicable to a range of temperatures much more vast.

**III. STRUCTURED [17] ALGORITHM TO THERMOCHEMICAL NON-EQUILIBRIUM**

Considering the three-dimensional and structured case, the algorithm follows that described in [21], considering, however, the vibrational contribution ([31]) and the version of the two-temperature model to the frozen speed of sound [Eq. (23)]. Hence, the discrete-dynamic-convective flux is defined by:

\[ R_{i+1/2,j,k} = [S]_{i+1/2,j,k} \left[ \frac{1}{2} M_{i+1/2,j,k} \right] \left[ \begin{array}{cc} \rho a & \rho a \\ \rho a & \rho a \\ \rho a & \rho a \\ \rho a & \rho a \\ \rho a & \rho a \end{array} \right] \left[ \begin{array}{cc} S_p \\ S_p \\ 0 \end{array} \right], \]  

(55)

the discrete-chemical-convective flux is defined by:

\[ R_{i+1/2,j,k} = [S]_{i+1/2,j,k} \left[ \frac{1}{2} M_{i+1/2,j,k} \right] \left( \begin{array}{c} \rho_{j}a \\ \rho_{j}a \\ \rho_{j}a \\ \rho_{j}a \\ \rho_{j}a \end{array} \right) \]  

(56)

and the discrete-vibrational-convective flux is determined by:

\[ R_{i+1/2,j,k} = [S]_{i+1/2,j,k} \left( \frac{1}{2} M_{i+1/2,j,k} \right) \left[ (pe_{a})_L + (pe_{a})_R \right] - \frac{1}{2} \phi_{i+1/2,j,k} \left[ (pe_{a})_R - (pe_{a})_L \right]. \]  

(57)
IV. RESULTS

Tests were performed in one personal computer Notebook with Dual Core Intel Pentium processor of 2.30 GHz of “clock” and 2.0 GBytes of RAM. As the interest of this work is steady state problems, it is necessary to define a criterion which guarantees the convergence of the numerical results. The criterion adopted was to consider a reduction of no minimal four (4) orders of magnitude in the value of the maximum residual in the calculation domain, a typical CFD-community criterion. The residual of each cell was defined as the numerical value obtained from the discretized conservation equations. As there are twelve (12) conservation equations to each cell, the maximum value obtained from these equations is defined as the residual of this cell. Hence, this residual is compared with the residual of the other cells, calculated of the same way, to define the maximum residual in the calculation domain. In the simulations, the attack angle was set equal to zero.

A. Initial and Boundary Conditions to the Studied Problem

The initial conditions are presented in Tab. 6. The Reynolds number is obtained from data of [35]. The boundary conditions to this problem of reactive flow are detailed in [24], as well the geometry in study, the meshes employed in the simulations and the description of the computational configuration.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(M_e)</td>
<td>8.78</td>
</tr>
<tr>
<td>(p_r)</td>
<td>0.00326 kg/m³</td>
</tr>
<tr>
<td>(\rho_r)</td>
<td>687 Pa</td>
</tr>
<tr>
<td>(U_e)</td>
<td>4,776 m/s</td>
</tr>
<tr>
<td>(T_e)</td>
<td>694 K</td>
</tr>
<tr>
<td>(T_{e,v})</td>
<td>694 K</td>
</tr>
<tr>
<td>altitude</td>
<td>40,000 m</td>
</tr>
<tr>
<td>(c_{NO})</td>
<td>10³</td>
</tr>
<tr>
<td>(c_{NO}^+)</td>
<td>0.05090</td>
</tr>
<tr>
<td>(c_{NO}^*)</td>
<td>0.0</td>
</tr>
<tr>
<td>(c_{N}^*)</td>
<td>0.0</td>
</tr>
<tr>
<td>(L)</td>
<td>2.0 m</td>
</tr>
<tr>
<td>(Re_c)</td>
<td>2.3885x10⁶</td>
</tr>
</tbody>
</table>

The geometry is a blunt body with 1.0 m of nose ratio and parallel rectilinear walls. The far field is located at 20.0 times the nose ratio in relation to the configuration nose. The dimensionless employed in the Euler and Navier-Stokes equations in this study are also described in [24].

B. Studied Cases

Table 7 presents the studied cases in this work, the mesh characteristics and the order of accuracy of the [17] scheme.
Table 7 Studied cases, mesh characteristics and accuracy order.

<table>
<thead>
<tr>
<th>Case</th>
<th>Mesh</th>
<th>Accuracy Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inviscid – 3D</td>
<td>63x60x10</td>
<td>First</td>
</tr>
</tbody>
</table>
| Viscous – 3D   | 63x60x10 (7.5%)
                      | First          |
| Inviscid – 3D | 63x60x10              | Second         |
| Viscous – 3D   | 63x60x10 (7.5%)       | Second         |

*Exponential stretching.

C. Results in Thermochemical Non-Equilibrium

*Inviscid, structured and first-order accurate case.* Figure 1 exhibits the pressure contours around the blunt body geometry calculated at the computational domain by the [17] scheme, in its first-order version, in thermochemical non-equilibrium. The non-dimensional pressure peak is equal to 148.46 unities and is located at the configuration nose. The solution presents good symmetry characteristics. Figure 2 shows the Mach number contours calculated at the computational domain. A region of subsonic flow is formed behind the normal shock wave, at the geometry nose. The shock wave develops normally: normal shock wave at the configuration nose, decaying to oblique shock waves and finally reaching, far from the blunt body, the Mach wave.

![Figure 1. Pressure contours.](image1)

Figure 1. Pressure contours.

Figure 3 presents the contours of the translational/rotational temperature distribution calculated at the computational domain. The translational/rotational temperature reaches a peak of 8,103 K at the configuration nose and determines an appropriated region to dissociation of N₂ and O₂. Along the blunt body, the translational/rotational temperature assumes an approximated value of 6,000 K, what also represents a good value to the dissociation firstly of O₂ and, in second place, of the N₂.

![Figure 3. T/R temperature contours.](image3)

Figure 3. T/R temperature contours.

Figure 4 exhibits the contours of the vibrational temperature calculated at the two-dimensional computational domain. Its peak reaches a value of 5,415 K and also contributes to the dissociation of N₂ and O₂, since the employed temperature to the calculation of the forward and backward reaction rates (reaction-rate-control temperature, T_{rrc}) in the thermochemical non-equilibrium is equal to $\sqrt{TV}$, the square root of the product between the translational/rotational temperature and the vibrational temperature.

![Figure 4. Vibrational temperature contours.](image4)

Figure 4. Vibrational temperature contours.
Hence, the effective temperature to the calculation of the chemical phenomena guarantees the couple between the vibrational mode and the dissociation reactions. In this configuration nose region, the temperature $T_{rrc}$ reaches, in the steady state condition, the approximated value of 6,624 K, assuring that the dissociation phenomena described above occurs. Good symmetry characteristics are observed.

Figure 5. Mass fraction distribution at the blunt body stagnation line.

Figure 5 shows the mass fraction distribution of the seven chemical species under study, namely: N, O, N$_2$, O$_2$, NO, NO$^+$ and e$, along the geometry stagnation line or geometry symmetry line. As can be observed from this figure, enough dissociation of N$_2$ and O$_2$ occur, with the consequent meaningful increase of N and of NO in the gaseous mixture. As mentioned early, this behaviour is expected due to the effective peak temperature reached at the calculation domain. The NO presented the biggest absolute increase in its formation, whereas the N presented the biggest relative increase. The O has not a meaningful increase due to the formation of the NO$^+$. The formation of e$^-$ is also discrete.

Viscous, structured and first-order accurate case. Figure 7 shows the Mach number contours calculated at the computational domain. The subsonic flow region, which is formed behind the normal shock, is well captured and propagates by the lower and upper geometry walls, due to the transport phenomena considered in the viscous simulations. The shock wave presents the expected behaviour: normal shock wave at the configuration nose, oblique shock waves and a Mach wave far from the blunt body.

Figure 8 exhibits the distribution of the translational/rotational temperature calculated at the computational domain. The peak of translational/rotational temperature reaches the approximated value of 8,797 K at the configuration nose and this value is observed along the lower and upper surfaces of the geometry.

Figure 9 presents the vibrational temperature distribution calculated at the computational domain. Its peak, at the configuration nose, reaches an approximated value of 5,401 K. The effective temperature to the calculation of the dissociation and recombination reactions, $T_{rrc}$, is equal approximately to 6,893 K, which guarantees that processes of dissociation of O$_2$ and N$_2$ can be captured by the employed formulation.
This value of effective temperature to the viscous reactive simulations is superior to that obtained in the inviscid case. Good symmetry characteristics are observed in these figures.

**Figure 9.** Vibrational temperature contours.

Inviscid, structured and second-order accurate case. Figure 11 shows the pressure contours obtained by the inviscid simulation performed by the second-order [17] scheme employing a minmod non-linear flux limiter. The non-dimensional pressure peak is approximately equal to 146 unities, slightly inferior to the respective peak obtained by the first-order solution. This pressure peak occurs at the configuration nose. The solution presents good symmetry characteristics. Figure 12 presents the Mach number contours obtained at the computational domain. The subsonic region which is formed behind the normal shock wave is well characterized at the configuration nose. Good symmetry characteristics are observed. The shock wave presents the expected behavior, passing from a normal shock at the configuration stagnation line to a Mach wave far from the blunt body.

**Figure 11.** Pressure contours.

**Figure 12.** Mach number contours.

Inviscid, structured and second-order accurate case. Figure 13 exhibits the contours of the translational/rotational temperature distribution calculated at the computational domain. The translational/rotational temperature peak occurs at the configuration nose and is approximately equal to 8,278 K. Figure 14 presents the contours of the vibrational temperature distribution calculated at the computational domain. The vibrational temperature peak is approximately equal to 2,365 K and is observed at the configuration nose. The effective temperature to calculation of the reaction rates (reaction rate control temperature, \( T_{rrc} \)) is approximately equal to 4,425 K, which represents a
temperature capable to capture the dissociation phenomena of N$_2$ and O$_2$. Good symmetry characteristics are observed in both figures.

Figure 13. T/R temperature contours.

Figure 15 exhibits the mass fraction distribution of the seven chemical species under study, namely: N, O, N$_2$, O$_2$, NO, NO$^+$ and e, along the geometry stagnation line. As can be observed, discrete dissociation of N$_2$ and O$_2$ occur, with consequent discrete increase of the N and of the NO, with subsequent reduction of the O, in the gaseous mixture. This behaviour is expected due to the effective temperature peak reached at the computational domain to the calculation of thermochemo non-equilibrium and to a second-order numerical formulation, which behaves in a more conservative way (see [22]), providing minor dissociation of N$_2$ and O$_2$.

**Viscous, structured and second-order accurate case.** Figure 16 exhibits the pressure contours calculated at the computational domain to the studied configuration of blunt body. The non-dimensional pressure peak is approximately equal to 164 unities, less than the respective value obtained by the first-order solution. The shock is positioned closer to the blunt body due to the mesh stretching and the employed viscous-reactive formulation. Good symmetry characteristics are observed.

Figure 16. Pressure contours.

Figure 17. Mach number contour.
Figure 17 shows the Mach number contours obtained at the computational domain. The subsonic region behind the normal shock wave, at the stagnation line, is well captured by the solution. This region propagates along the lower and upper surfaces of the geometry, due to the transport phenomena (viscosity, thermal conductivity and species diffusion). The shock wave behaviour is also the expected: normal shock at the geometry nose, oblique shock waves close to the configuration and Mach wave far from the geometry.

![Figure 17. Mach number contours.](image)

Figure 17. Mach number contours obtained at the computational domain.

Figure 18 exhibits the translational/rotational temperature distribution calculated at the computational domain. The temperature peak at the configuration nose reaches approximately 8,491 K. Figure 19 shows the vibrational temperature distribution calculated at the computational domain. The temperature peak at the nose and along the lower and upper surfaces of the geometry is equal to 5,901 K. The effective temperature to the calculation of the reaction rates, \( T_{re} \), was of 7,079 K, superior to that obtained with the first-order solution, which is representative to the calculation of the \( \text{N}_2 \) and \( \text{O}_2 \) dissociations. Both Figs. 18 and 19 exhibit good symmetry characteristics.

![Figure 18. T/R temperature contours.](image)

Figure 18. T/R temperature contours.

Figure 19. Vibrational temperature contours.

![Figure 19. Vibrational temperature contours.](image)

Figure 19. Vibrational temperature contours.

Figure 20 presents the mass fraction distribution of the seven chemical species under study, namely: N, O, \( \text{N}_2 \), \( \text{O}_2 \), NO, NO\(^+\) and \( \text{e}^- \), along the geometry stagnation line. As can be observed, good dissociation of \( \text{N}_2 \) and \( \text{O}_2 \) occur, with consequent good increase of N and NO in the gaseous mixture. This behavior is expected due to the effective temperature peak reached at the computational domain to the calculation of thermochemical non-equilibrium and to a second-order numerical formulation, which behaves in a more conservative way ([22]), providing major dissociation of \( \text{N}_2 \) and \( \text{O}_2 \). In other words, this solution provided by the second-order [17] scheme, as seen in other cases, tends to provide bigger dissociation of \( \text{N}_2 \) and \( \text{O}_2 \). As this solution is more precise (second-order), it should be considered as standard to comparison with other schemes. The NO\(^+\) is formed with the subsequent reduction of the O species.

![Figure 20. Mass fraction distribution at the blunt body stagnation line.](image)

Figure 20. Mass fraction distribution at the blunt body stagnation line.

**Shock Position.** In this section is presented the behaviour of the shock position in thermochemical non-equilibrium conditions for the five and seven species models. Both first- and second-order solutions are compared between them.

![Figure 31. Shock position (inviscid).](image)

Figure 31. Shock position (inviscid).

The detached shock position in terms of pressure distribution, in the inviscid case, and first- and second-order...
accurate solutions, is exhibited in Fig. 31. It is shown the thermochemical non-equilibrium shock position for the five and seven species models. As can be observed, the second-order results yield closer shock positions in relation to the blunt body nose. Particularly, the second-order, five species model, is the closest solution to the inviscid case.

Table 9 compares the values obtained from the simulations with this theoretical parameter and presents the numerical percentage errors. As can be observed, all solutions present percentage errors less than 20%, which is a reasonable estimation of the stagnation pressure.

Another possibility to quantify the results is the determination of the shock standoff distance. [37] presents a graphic in which is plotted the shock standoff distance of a pre-determined configuration versus the Mach number. Considering the blunt body nose approximately as a cylinder and using the value 8.78 to the Mach number, it is possible to obtain the value 0.19 to the ratio \( \delta/d \), where \( \delta \) is the position of the normal shock wave in relation to the body nose and \( d \) is a characteristic length of the configuration. In the present study, \( d = 2.0 \text{m} \) (diameter of the body nose) and \( \delta = 0.38 \text{m} \). Table 10 presents the values obtained by \( \delta \) for the different cases and the percentage errors. This table shows that the best result is obtained with the structured, viscous, second order version of [17]. As the shock standoff distance presented in [37] is more realistic, presenting smaller dependence of the perfect gas hypothesis, improved results were expected to obtain in this study. Hence, the best solution is obtained by the [17] scheme in its second order version.

**Table 9 Comparisons between theoretical and numerical results.**

<table>
<thead>
<tr>
<th>Case</th>
<th>( p_{r0} )</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inviscid/Structured/1st Order</td>
<td>148.46</td>
<td>17.11</td>
</tr>
<tr>
<td>Viscous/Structured/1st Order</td>
<td>170.00</td>
<td>5.08</td>
</tr>
<tr>
<td>Inviscid/Structured/2nd Order</td>
<td>145.76</td>
<td>18.62</td>
</tr>
<tr>
<td>Viscous/Structured/2nd Order</td>
<td>164.36</td>
<td>8.23</td>
</tr>
</tbody>
</table>

**Table 10 Shock standoff distance obtained from numerical schemes.**

<table>
<thead>
<tr>
<th>Case</th>
<th>( \delta_{\text{NUM}} ) (m)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inviscid/Structured/1st Order</td>
<td>0.80</td>
<td>110.53</td>
</tr>
<tr>
<td>Viscous/Structured/1st Order</td>
<td>0.48</td>
<td>26.32</td>
</tr>
<tr>
<td>Inviscid/Structured/2nd Order</td>
<td>0.60</td>
<td>57.89</td>
</tr>
<tr>
<td>Viscous/Structured/2nd Order</td>
<td>0.40</td>
<td>5.26</td>
</tr>
</tbody>
</table>

**Computational performance of the studied algorithms.** Table 11 presents the computational data of the reactive simulations performed with the [17] scheme to the problem of the blunt body in three-dimensions. The reactive simulations involved the thermochemical non-equilibrium solutions obtained from five [47] and seven chemical species.

In this table are exhibited the studied case, the maximum number of CFL employed in the simulation, the number of iterations to convergence and the number of orders of reduction in the magnitude of the maximum residual in relation to its initial value.
The implementation of an unstructured generator, which was not the objective of the present work, and to obtain a generalized algorithm to the solution of the reactive equations.

In this work, first part of this study, the structured formulation of the three-dimensional Euler and Navier-Stokes reactive equations is presented. In [40], the second part of this study, it will be presented the unstructured version of the calculation algorithm in three-dimensions to complete the formulation in structured and in unstructured contexts.

The reactive simulations involved an air chemical model of seven species: N, O, N$_2$, O$_2$, NO, NO$^+$ and e$^-$. Eighteen chemical reactions, involving dissociation, recombination and ionization, were simulated by the proposed model. This model was suggested by [46]. The Arrhenius formula was employed to determine the reaction rates and the law of mass action was used to determine the source terms of each gas specie equation.

The results have demonstrated that the most correct aerodynamic coefficient of lift is obtained by the [17] scheme with first-order accuracy, in an inviscid formulation, to a five species model. The cheapest algorithm was due to [17], inviscid, first-order accurate, structured, and five species model. Moreover, the shock position is closer to the geometry as using the reactive formulation than the ideal gas formulation. It was verified in [22]. Comparing the five species model and the seven species model, the second order solution of both models present the best behaviour. Errors less than 20% were obtained with this version of the [17] algorithm in the determination of the stagnation pressure at the body nose and an error of 7.89% was found in the determination of the shock standoff distance, highlighting the correct implementation and good results obtained from the reactive formulation. Values of these parameters were evaluated and proved the significant potential of the present numerical tool.

This work, as also [40], is the continuation of the study started at [41], based on the work of [42]. Other references on the non-equilibrium reactive flows area are: [43], [44] and [45].

V. CONCLUSION

This work, the first part of this study, presents a numerical tool implemented to simulate inviscid and viscous flows employing the reactive gas formulation of thermochemical nonequilibrium flow in three-dimensions. The Euler and Navier-Stokes equations, employing a finite volume formulation, on the context of structured and unstructured spatial discretizations, are solved. These variants allow an effective comparison between the two types of spatial discretization aiming verify their potentialities: solution quality, convergence speed, computational cost, etc. The aerospace problem involving the “hot gas” hypersonic flow around a blunt body, in three-dimensions, is simulated.

To the simulations with unstructured spatial discretization, a structured mesh generator developed by the first author ([38]), which creates meshes of hexahedrons (3D), was employed. After that, as a pre-processing stage ([39]), such meshes were transformed in meshes of tetrahedrons. Such procedure aimed to avoid the time which would be waste with the

Table 11 Computational data of the reactive simulations with the 2D blunt body.

<table>
<thead>
<tr>
<th>Studied case</th>
<th>CFL</th>
<th>Iterations</th>
<th>Orders of Residual Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>First-Order / Structured / Inviscid / FS$^{(a)}$</td>
<td>0.9</td>
<td>373</td>
<td>4</td>
</tr>
<tr>
<td>First-Order / Structured / Viscous / FS</td>
<td>0.7</td>
<td>1,005</td>
<td>4</td>
</tr>
<tr>
<td>Second-Order / Structured / Inviscid / FS</td>
<td>0.3</td>
<td>982</td>
<td>4</td>
</tr>
<tr>
<td>Second-Order / Structured / Viscous / FS</td>
<td>0.3</td>
<td>2,412</td>
<td>4</td>
</tr>
<tr>
<td>First-Order / Structured / Inviscid / SS$^{(b)}$</td>
<td>0.9</td>
<td>372</td>
<td>4</td>
</tr>
<tr>
<td>First-Order / Structured / Viscous / SS</td>
<td>0.7</td>
<td>997</td>
<td>4</td>
</tr>
<tr>
<td>Second-Order / Structured / Inviscid / SS</td>
<td>0.1</td>
<td>2,908</td>
<td>4</td>
</tr>
<tr>
<td>Second-Order / Structured / Viscous / SS</td>
<td>0.7</td>
<td>1,173</td>
<td>4</td>
</tr>
</tbody>
</table>

$^{(a)}$: Five Species; $^{(b)}$: Seven Species.

As can be observed, all test-cases converged with no minimal four orders of reduction in the value of the maximum residual. The maximum numbers of CFL presented the following distribution: 0.9 in two (2) cases (25.00%), 0.7 in three (3) cases (37.50%), 0.3 in two (2) cases (25.00%) and 0.1 in one (1) case (12.50%). The convergence iterations did not overtake 3,000, in all studied cases. However, the time wasted in the simulations was much raised, taking until days to convergence (to four orders of reduction in the maximum residual). It is important to emphasize that all two-dimensional viscous simulations were considered laminar, without the introduction of a turbulence model, although high Reynolds number were employed in the simulations.

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Edisson S. G. Maciel (F’14), born in 1969, February 25, in Recife, Pernambuco. He is a Mechanical Engineering undergraduated by UFPE in 1992, in Recife, PE, Brazil; Mester degree in Thermal Engineering by UFPE in 1995, in Recife, PE, Brazil; Doctor degree in Aeronautical Engineering by ITA in 2002, in São José dos Campos, SP, Brazil; and Post-Doctor degree in Aeronautical Engineering by ITA in 2009, in São José dos Campos, SP, Brazil.