Turbulent Thermochemical Non-Equilibrium Reentry Flows in 2D

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Citation

Abstract
In this work, a study involving the fourth-order ENO procedure using the Newton interpolation process from Harten et al. is presented. The Favre averaged Navier-Stokes equations, in conservative and finite volume contexts, employing structured spatial discretization, are studied. Turbulence is taken into account considering the implementation of three k-ω two-equation turbulence models, based on the works of Coakley, Wilcox, and Yoder, Georgiadis and Orkwis. The results have indicated that the Yoder, Georgiadis and Orkwis turbulence model yields the best prediction of the stagnation pressure value, although the Coakley turbulence model is more computationally efficient.

1. Introduction

Renewed interest in the area of hypersonic flight has brought computational fluid dynamics (CFD) to the forefront of fluid flow research [1]. Many years have seen a quantum leap in advancements made in the areas of computer systems and software which utilize them for problem solving. Sophisticated and accurate numerical algorithms are devised routinely that are capable of handling complex computational problems. Experimental test facilities capable of addressing complicated high-speed flow problems are still scarce because they are too expensive to build and sophisticated measurements techniques appropriate for such problems, such as the non-intrusive laser, are still in the development stage. As a result, CFD has become a vital tool, in some cases the only tool, in the flow research today.

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 [2-3].

In spite of the advances made in the area of compressible turbulence modeling in recent years, no universal turbulence model, applicable to such complex flow problems has emerged so far. While the model should be accurate it should also be economical to use in conjunction with the governing equations of the fluid flow. Taking these issues into consideration, k-ω two-equation models have been chosen in the present work [4, 5, 6]. These models solve differential equations for the turbulent kinetic energy and the vorticity. Additional differential equations for the variances of temperature and species mass fractions have also been included. These variances have been used to model the turbulence-chemistry interactions in the reacting flows studied here.
Harten et al. and other researchers [7-12] developed in recent years the so called Essentially Non-Oscillatory (ENO) schemes, which have uniform high order of accuracy outside discontinuities. The main feature of ENO schemes is that they use an adaptive stencil. At each grid cell or point a searching algorithm determines which part of the flow surrounding that grid cell or point is the smoothest. This stencil is then used to construct a high order accurate, conservative interpolation to determine the variables at the cell faces. This interpolation process can be applied to conservative variables, characteristic variables, or the fluxes, either defined as cell averaged or point values. The ENO scheme tries to minimize numerical oscillations around discontinuities by using predominantly data from the smooth parts of the flow field. Due to the constant stencil switching the ENO scheme is highly non-linear and only limited theoretical results are available ([7-8]).

In this work, a study involving the fourth-order ENO procedure using the Newton interpolation process from [9] is presented. The Favre averaged Navier-Stokes equations, in conservative and finite volume contexts, employing structured spatial discretization, are studied. The ENO procedure is presented to a conserved variable interpolation process, using the Newton method, to fourth-order of accuracy. Turbulence is taken into account considering the implementation of three k-ω two-equation turbulence models, based on the works of [4, 5, 6]. The numerical algorithm of [13] is used to perform the reentry flow numerical experiments. The “hot gas” hypersonic flow around a blunt body, in two-dimensions, is simulated. The convergence process is accelerated to steady state condition through a spatially variable time step procedure, which has proved effective gains in terms of computational acceleration ([14-15]). The reactive simulations involve Earth atmosphere chemical models of five species and seventeen reactions, based on the [16] model, and seven species and eighteen reactions, based on the [17] model. The results have indicated that the [15] turbulence model yields the best prediction of the stagnation pressure value, although the [13] turbulence model is more computationally efficient.

2. Favre Average

The Navier-Stokes equations and the equations for energy and species continuity which governs the flows with multiple species undergoing chemical reactions have been used [18-20] for the analysis. Details of the present implementation for each chemical model, the specification of the thermodynamic and transport properties, as well the vibrational model are described in [21-24]. Density-weighted averaging [25] is used to derive the turbulent flow equations from the above relations. The dependent variables, with exception of density and pressure, are written as,

\[
\phi = \bar{\phi} + \phi^* , \tag{1}
\]

where the \( \phi^* \) is the fluctuating component of the variable under consideration and its Favre-mean \( \bar{\phi} \) is defined as

\[
\bar{\phi} = \frac{\rho \phi}{\bar{\rho}} . \tag{2}
\]

In this equation, the overbar indicates conventional time-averaging. Density and pressure are split in the conventional sense as,

\[
\rho = \bar{\rho} + \rho^* \quad \text{and} \quad p = \bar{p} + \rho^* . \tag{3}
\]

The average continuity and momentum equations are

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{U}_i}{\partial x_j} = 0 ; \tag{4}
\]

\[
\frac{\partial \bar{p} \bar{U}_i}{\partial t} + \frac{\partial \bar{p} \bar{U}_j}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{u}_j \bar{u}_i}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} , \tag{5}
\]

where:

\[
\tau_{ij} = \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) , \tag{6}
\]

with repeated indices indicating summation. The mass-averaged total energy can be written in terms of the total enthalpy as

\[
\frac{\bar{e}}{\bar{p}} = \bar{H} - \frac{\bar{p}}{\bar{p}} . \tag{7}
\]

Using the above definition and omitting the body force contribution, the time-averaged energy equation is

\[
\frac{\partial \bar{e}}{\partial t} + \frac{\partial (\bar{e} + \bar{p}) \bar{U}_j}{\partial x_j} = - \frac{\partial \bar{q}_j}{\partial x_j} + \frac{\partial \bar{u}_j \tau_{ij}}{\partial x_j} - \frac{\partial \bar{p} \bar{u}_j}{\partial x_j} , \tag{8}
\]

where \( \bar{q}_j \) represents the averaged heat flux term. The species conservation equation is

\[
\frac{\partial \bar{c}_j}{\partial t} + \frac{\partial (\bar{c} \bar{U}_j)}{\partial x_j} = \bar{\omega}_j - \frac{\partial (\bar{p} \bar{u}_j c_j' + \rho \bar{c}_j \bar{V}_j)}{\partial x_j} . \tag{9}
\]

The equations for the two turbulence variables, turbulent kinetic energy (k) and vorticity (ω) are derived using the momentum and continuity equations and time-averaging [26-27]. These equations are presented in the fourth section.

3. Modelled Equations

Closure of the averaged equations is achieved by invoking the Boussinesq approximation in which relates the turbulent stresses (Reynolds stresses) to the mean strain rate. The Reynolds stress tensor is written as,
\[
\begin{align*}
-\rho u_i U_j &= \mu_T \frac{\partial^2 \phi}{\partial x_j} - \frac{2}{3} \rho k \delta_{ij} \\
S_j &= \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} 
\end{align*}
\]

(10)

where \( \mu_T \) is the turbulent/eddy viscosity and its definition depends on the construction of the studied k-\( \omega \) model.

The correlation between fluctuating velocity and the scalar fluctuations are modelled in a similar manner using a mean gradient hypothesis. A typical model is,

\[
-\rho u_i \phi^r = \mu_T \frac{\partial^2 \phi}{\partial x_j} 
\]

(11)

where \( \sigma_\phi \) is a coefficient which, normally, is a constant. For \( \phi \)

\[
\frac{\partial c_i}{\partial t} + \frac{\partial (\bar{u} \cdot \bar{c})}{\partial x_j} = \frac{\partial \left( \tau_{ij} - \rho u_i u_j \right)}{\partial x_j} + \frac{\partial \left( \frac{\tau_i}{\sigma_e} \right)}{\partial x_j}.
\]

(15)

Differential equations for the variances of static enthalpy and species mass fractions have also been introduced in the solutions. Equations for \( h^2 \) and \( c_i c_i^{\prime} \) have been derived. The modelled equations take a similar form as that of the turbulent kinetic energy (to be seen in the next section). These equations are given below.

\[
\begin{align*}
\frac{\partial \rho g}{\partial t} + \frac{\partial \rho g U_j}{\partial x_j} &= -2 \rho u_i G \frac{\partial \phi}{\partial x_j} + \frac{\partial \left( \frac{\tau_i}{\sigma_e} \right)}{\partial x_j} + \Psi, \\
\end{align*}
\]

(16)

where for \( g = h^2 \), \( G = \bar{h} \), \( \Psi = 0 \), \( \sigma = \text{Pr}_d \) and \( \sigma_\phi = \text{Sc}_T \),

\[
\omega_e = M \sum_{i=1}^{n_s} \left( v_i - v_j \right) \left\{ k_{p_i} d^n \prod_{i=1}^{n_s} \left( \frac{c_i}{M_i} \right)^{v_i} - k_{p_i} d^n \prod_{i=1}^{n_s} \left( \frac{c_i}{M_i} \right)^{v_i} \right\},
\]

(17)

and this equation is solved instead of the individual species variance equations. The production term [first term on the right hand side of Eq. (16)] is evaluated using Eq. (11).

In a system involving \( I \) reaction steps and \( N \) species, the instantaneous production rate of a scalar \( i \) can be represented – from the law of mass action – in the following general form:

\[
k_{ij} = A_i T^{b_i} \exp \left(-\frac{T_{aj}}{T}\right),
\]

(19)

where \( A_i, b_i \) and \( T_{aj} \) are numerical constants specific to the given reaction.

The purpose of solving the \( g \)-equations is to include the interaction between turbulence and chemical reactions in the reacting flow cases. The effect of temperature fluctuations on the species production rate is included using an approximate analysis. Here the Arrhenius equations for the reaction rate term is written in terms of mean and fluctuating components of the temperature and expanded in the form of a series. The terms are truncated at the second order level of the fluctuations and the calculated variance of temperature is used to evaluate the resultant reaction rate term. The reaction rate term is given by the Arrhenius rate equation [Eq. (19)].
mean temperature is approximately 0.6 and this is the value adopted in this work.

Practical reactive flows involve multiple scalar mixing and reactions. For such flows, [28] suggests the use of a multivariate β-pdf model to account for the effects of the scalar fluctuations on the species production rates. This model is briefly outlined below. The multivariate β-pdf for the N-scalar mixing process is given by

\[ F(f) = \prod_{i=1}^{N} (\beta_{1i} + \cdots + \beta_{Ni}) \prod_{i=1}^{N} (1 - \beta_{1i} - \cdots - \beta_{Ni}) \]  

(24)

The parameters of the model \((\beta_{1i}, \ldots, \beta_{Ni})\) are functions of the mean mass fractions \(\bar{c}_i\) and turbulent scalar energy \(Q_s\) [Eq. (17):]

\[ \beta_i = \bar{c}_i \left(1 - \frac{Q_s}{\tilde{Q}_s} - 1\right) \]  

(25)

where \(S\) is given by

\[ S = \sum_{i=1}^{N} \bar{c}_i^2 \]  

(26)

Subject to the above simplifications the mean species production rate is given by,

\[ \dot{\omega}_l = M_i \sum_{i=1}^{N} (\bar{v}_{ij} - \bar{v}_j) \left\{ \bar{k}_ij \rho^m \left[ \prod_{i=1}^{N}(M_i)^{\bar{v}_i} \right] \bar{I}_{ij} - \bar{k}_ij \rho^n \left[ \prod_{i=1}^{N}(M_i)^{\bar{v}_i} \right] I_{bj} \right\}, \]  

(27)

where:

\[ m = \left[ b \left( \frac{b + \frac{\bar{T}_a}{\bar{T}}}{2} \right) + \frac{1}{2} \left( \frac{\bar{T}_a}{\bar{T}} \right)^2 \right] \frac{\bar{T}_a}{\bar{T}}. \]  

(23)

The terms \(I_{j}\) and \(I_{bj}\) are also moments of the scalar joint-pdf, and can be easily evaluated as

\[ I_{j} = \prod_{i=1}^{N} \bar{c}_i^{\bar{v}_j} \quad \text{and} \quad I_{bj} = \prod_{i=1}^{N} \bar{c}_i^{\bar{v}_j}. \]  

(28)

The expression for \(I_{j}\) is

\[ I_{j} = \prod_{i=1}^{N} \left( \beta_i + \bar{v}_{ij} - \bar{v}_j \right) \prod_{p=1}^{m_j} (B + m_j - p). \]  

(29)

In the above equations, angular brackets represent conventional time averaging. The expression for \(I_{j}\) is [36],

\[ I_{j} = \sum_{i=1}^{N} \bar{c}_i \sum_{k=1}^{N} \prod_{i=1}^{\bar{v}_j} \left( \beta_i + \bar{v}_{ij} - \bar{v}_j \right) \prod_{j=1}^{m_j} (B + m_j - p). \]  

(30)

Similarly, the expression for \(I_{bj}\) is,

\[ I_{bj} = \prod_{i=1}^{N} \prod_{j=1}^{\bar{v}_j} \left( \beta_i + \bar{v}_{ij} - \bar{v}_j - \bar{v}_j \right) \prod_{p=1}^{n_j} (B + n_j - p). \]  

(31)

The expression for the source term in the scalar variance \(Q_s\) is given by [36],

\[ \sum_{i=1}^{N} \bar{c}_i \bar{c}_i = \sum_{i=1}^{N} \sum_{j=1}^{\bar{v}_j} \left( \bar{v}_{ij} - \bar{v}_j \right) \left\{ \bar{k}_ij \rho^m \left[ \prod_{i=1}^{N}(M_i)^{\bar{v}_i} \right] \bar{J}_j - \bar{k}_ij \rho^n \left[ \prod_{i=1}^{N}(M_i)^{\bar{v}_i} \right] J_{bj} \right\}, \]  

(32)

with

\[ J_{j} = \bar{c}_i \prod_{i=1}^{N} \bar{c}_i^{\bar{v}_j} \quad \text{and} \quad J_{bj} = \bar{c}_i \prod_{i=1}^{N} \bar{c}_i^{\bar{v}_j}. \]  

(33)
4. Navier-Stokes Equations

The flow is modelled by the Favre-averaged Navier-Stokes equations and the condition of thermochemical non-equilibrium, where the rotational and vibrational contributions are considered, is taken into account. Only the reactive Navier-Stokes equations for the five species model is exhibited, although the seven species model could be obtained including more two species equations and adjusting the respective terms to this formulation. Details of the five species model and seven species model implementation are described in [21-24], and the interested reader is encouraged to read these works to become aware of the present study.

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

$$\frac{\partial}{\partial t} \int_Q Q dV + \int_{\partial S} \vec{F} \cdot \vec{n} dS + \int_V G dV = \int_{S_{CV}} e h dV,$$

where: $Q$ is the vector of conserved variables, $V$ is the volume of a computational cell, $\vec{F}$ is the complete flux vector, $\vec{n}$ is the unity vector normal to the flux face, $S$ is the flux area, $G$ is the k-\(\omega\) two-equation model source term, $S_{CV}$ is the chemical and vibrational source term, $E_x$ and $E_y$ are the convective flux vectors or the Euler flux vectors in the x and y directions, respectively. $E_\ell$ and $F_\ell$ are the viscous flux vectors in the x and y directions, respectively. The $\vec{i}$ and $\vec{j}$ unity vectors define the Cartesian coordinate system. Thirteen (13) conservation equations are solved: one of general mass conservation, two of linear momentum conservation, one of total energy, four of species mass conservation, one of the vibrational internal energy of the molecules, two of the k-\(\omega\) turbulence model, and two of the g-equations. Therefore, one of the species is absent of the iterative process. The CFD 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, the $N_2$ was chosen. The vectors $Q$, $E_x$, $F_x$, $E_y$, $F_y$, $G$ and $S_{CV}$ can, hence, be defined as follows:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho_1 \\ \rho_{1u} \\ \rho_{1v} \\ \rho_2 \\ \rho_{2u} \\ \rho_{2v} \\ e_v \\ \rho_{e_v} \\ pk \\ p\omega \end{bmatrix}, \quad E_x = \begin{bmatrix} p u \\ \rho u^2 + p \\ \rho uv \\ \rho Hv \\ \rho_{1u} \\ \rho_{1v} \\ \rho_{2u} \\ \rho_{2v} \\ \rho v \\ \rho_{e_v} \\ \rho_{e_v} \\ \rho v \omega \end{bmatrix},$$

$$E_y = \begin{bmatrix} 0 \\ \rho v \\ \rho uv \\ \rho Hv \\ \rho_{2v} \\ \rho_{2v} \\ \rho_{e_v} \\ \rho_{e_v} \\ \rho_{e_v} \\ \rho v \omega \end{bmatrix},$$

$$F_x = \begin{bmatrix} 0 \\ t_{xx} + \tau_{xx} \\ t_{xy} + \tau_{xy} \\ f_{x} - \phi_{x} \\ -\rho_{v_{xx}} - \theta_{xx} \\ -\rho_{v_{xy}} - \theta_{xy} \\ -\rho_{v_{xx}} - \theta_{xx} \\ -\rho_{v_{xy}} - \theta_{xy} \\ \alpha_{x} \\ \beta_{x} \\ \gamma_{x} \\ \delta_{x} \end{bmatrix},$$

$$F_y = \begin{bmatrix} 0 \\ t_{yy} + \tau_{yy} \\ t_{xy} + \tau_{xy} \\ f_{y} - \phi_{y} \\ -\rho_{v_{yy}} - \theta_{yy} \\ -\rho_{v_{xy}} - \theta_{xy} \\ -\rho_{v_{yy}} - \theta_{yy} \\ -\rho_{v_{xy}} - \theta_{xy} \\ \alpha_{y} \\ \beta_{y} \\ \gamma_{y} \\ \delta_{y} \end{bmatrix},$$

in which: $\rho$ is the mixture density; $u$ and $v$ are Cartesian components of the velocity vector in the x and y directions, respectively; $p$ is the fluid static pressure; $e$ is the fluid total energy; $\rho_1$, $\rho_2$, $\rho_4$ and $\rho_5$ are densities of the N, O, O$_2$ and NO, respectively; the $\tau$’s are the components of the Reynolds stress tensor; the $f$‘s are the components of the viscous stress tensor; $f_{x}$ and $f_{y}$ are viscous work and Fourier heat flux functions; $\rho_{v_{xx}}$ and $\rho_{v_{xy}}$ represent the species diffusion flux, defined by the Fick law; $\phi_{x}$ and $\phi_{y}$ are the terms of mixture diffusion; $\phi_{\gamma_x}$ and $\phi_{\gamma_y}$ are the terms of molecular diffusion calculated at the vibrational temperature; $k$ is the turbulent kinetic energy; $\omega$ is the turbulent vorticity;
The viscous stresses, in N/m², are determined, according to a Newtonian fluid model, by:

\[
\begin{align*}
t_{xx} &= \left[ 2\mu_M \frac{\partial u}{\partial x} - 2/3 \mu_M \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right]; \\
t_{xy} &= \mu_M \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right); \\
t_{yy} &= \left[ 2\mu_M \left( \frac{\partial v}{\partial y} - 2/3 \mu_M \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right].
\end{align*}
\]

The components of the turbulent stress tensor (Reynolds stress tensor) are described by the following expressions:

\[
\begin{align*}
\tau_{xx} &= \left[ 2\mu_T \frac{\partial u}{\partial x} - 2/3 \mu_T \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] - 2/3 \Re Pr k; \\
\tau_{xy} &= \mu_T \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right); \\
\tau_{yy} &= \left[ 2\mu_T \frac{\partial v}{\partial y} - 2/3 \mu_T \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] - 2/3 \Re Pr k.
\end{align*}
\]

Expressions to \( f_x \) and \( f_y \) are given bellow:

\[
\begin{align*}
f_x &= \left( t_{xx} + \tau_{xx} \right) u + \left( t_{xy} + \tau_{xy} \right) v + q_v + q_h + k_x; \\
f_y &= \left( t_{xy} + \tau_{xy} \right) u + \left( t_{yy} + \tau_{yy} \right) v + q_v + q_h + k_y,
\end{align*}
\]

where \( q_v \) and \( q_h \) are the Fourier heat flux components and are given by:

\[
\begin{align*}
q_x &= \mu_M / \Pr L + \mu_T / \Pr_T \partial h / \partial x; \\
q_y &= \mu_M / \Pr L + \mu_T / \Pr_T \partial h / \partial y.
\end{align*}
\]

with \( \mu_M \) being the molecular viscosity and \( \Pr L \), the laminar Prandtl number. The \( q_v \) and \( q_h \), are the vibrational heat flux components and are given by:

\[
\begin{align*}
q_v &= k_v \partial T_v / \partial x; \\
q_h &= k_v \partial T_v / \partial y.
\end{align*}
\]

with \( k_v \) being the vibrational thermal conductivity and \( T_v \) is the vibrational temperature, what characterizes this model as of two temperatures: translational/rotational and vibrational. The last terms in Eqs. (42)-(43) are \( k_x \) and \( k_y \) and are defined as follows:

\[
\begin{align*}
k_x &= \left( \mu_M + \mu_T / \sigma_k \right) \partial k / \partial x; \\
k_y &= \left( \mu_M + \mu_T / \sigma_k \right) \partial k / \partial y.
\end{align*}
\]

The diffusion terms related to the \( k-\omega \) equations are defined as:

\[
\begin{align*}
\alpha_x &= \left( \mu_M + \mu_T / \sigma_k \right) \partial \omega / \partial x; \\
\alpha_y &= \left( \mu_M + \mu_T / \sigma_k \right) \partial \omega / \partial y; \\
\beta_x &= \left( \mu_M + \mu_T / \sigma_a \right) \partial \omega / \partial x; \\
\beta_y &= \left( \mu_M + \mu_T / \sigma_a \right) \partial \omega / \partial y; \\
\gamma_x &= \left( \mu_M / \Pr_L + \mu_T / \Pr_T \right) \partial Q_h / \partial x; \\
\gamma_y &= \left( \mu_M / \Pr_L + \mu_T / \Pr_T \right) \partial Q_h / \partial y.
\end{align*}
\]
\[
\delta_x = \left(\frac{\mu_M}{Sc} + \mu_T/Sc_T\right)\partial Q_s/\partial x;
\]
\[
\delta_y = \left(\frac{\mu_M}{Sc} + \mu_T/Sc_T\right)\partial Q_s/\partial y;
\]
(52)

The terms of species diffusion, defined by the Fick law, to a condition of thermal non-equilibrium, are determined by ([29]):
\[
\rho_{s}v_{sx} = -\rho D_s \frac{\partial Y_{MF,s}}{\partial x} \quad \text{and} \quad \rho_{s}v_{sy} = -\rho D_s \frac{\partial Y_{MF,s}}{\partial y},
\]
(53)
with “s” referent to a given species, \(Y_{MF,s}\) being the molar fraction of the species, defined as:
\[
Y_{MF,s} = \frac{\rho_s}{\sum_k \rho_k / M_k}
\]
(54)
and \(D_s\) is the species-effective-diffusion coefficient.

The diffusion terms \(\delta_x\) and \(\delta_y\), which appear in the energy equation are defined by ([16]):
\[
\phi_x = \sum_{s=1}^{n_s} \rho_s v_{sx} h_{s} \quad \text{and} \quad \phi_y = \sum_{s=1}^{n_s} \rho_s v_{sy} h_{s},
\]
(55)
being \(h_{s}\) the specific enthalpy (sensible) of the chemical species “s”. The molecular diffusion terms calculated at the vibrational temperature, \(\phi_{sx}\) and \(\phi_{sy}\), which appear in the vibrational-internal-energy equation are defined by ([29]):
\[
\phi_{v,x} = \sum_{s=\text{mol}} \rho_s v_{sx} h_{v,s} \quad \text{and} \quad \phi_{v,y} = \sum_{s=\text{mol}} \rho_s v_{sy} h_{v,s},
\]
(56)
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. (56), as also those present in Eq. (38), considers only the molecules of the system, namely: \(N_2, O_2\) and \(NO\).

Finally, the \(\theta\)‘s terms of Eq. (37) are described as,
\[
\theta_{sx} = \left(\frac{\mu_M}{Sc} + \mu_T/Sc_T\right)\partial c_s /\partial x;
\]
(57)
\[
\theta_{sy} = \left(\frac{\mu_M}{Sc} + \mu_T/Sc_T\right)\partial c_s /\partial y.
\]
(58)

5. Flux Vector Splitting Scheme

Considering the two-dimensional and structured case, the algorithm follows that described in [21-24]. The system is solved in three parts separately, according to [30]. The first part takes into account the dynamic part, which considers the Navier-Stokes equations plus the turbulence equations, the second one takes into account the chemical part, and the third part takes into account the vibrational part. Hence, the discrete-dynamic-convective flux, which solves the dynamic and turbulent parts, is given by:

\[
R_{i+1/2,j} = |S|_{i+1/2,j} \left[ \begin{array}{c}
\rho_a \\
p_a \\
pav \\
pav \\
pavH \\
pavH \\
pato \\
pQ \end{array} \right] + \frac{1}{2} \left[ \begin{array}{c}
\rho_{a}^L \\
p_{a}^L \\
pav_{a}^L \\
pav_{a}^L \\
pavH_{a}^L \\
pavH_{a}^L \\
pato_{a}^L \\
pQ_{a}^L \end{array} \right] - \frac{1}{2} q_{i+1/2,j} \left[ \begin{array}{c}
\rho_{a}^R \\
p_{a}^R \\
pav_{a}^R \\
pav_{a}^R \\
pavH_{a}^R \\
pavH_{a}^R \\
pato_{a}^R \\
pQ_{a}^R \end{array} \right],
\]
(59)

the discrete-chemical-convective flux is defined by:
\[
R_{i+1/2,j} = |S|_{i+1/2,j} \left[ \begin{array}{c}
\rho_{a} \\
p_{a} \\
pav \\
pav \\
pavH \\
pavH \\
pato \\
pQ \end{array} \right] + \frac{1}{2} \left[ \begin{array}{c}
\rho_{a}^L \\
p_{a}^L \\
pav_{a}^L \\
pav_{a}^L \\
pavH_{a}^L \\
pavH_{a}^L \\
pato_{a}^L \\
pQ_{a}^L \end{array} \right] - \frac{1}{2} q_{i+1/2,j} \left[ \begin{array}{c}
\rho_{a}^R \\
p_{a}^R \\
pav_{a}^R \\
pav_{a}^R \\
pavH_{a}^R \\
pavH_{a}^R \\
pato_{a}^R \\
pQ_{a}^R \end{array} \right],
\]
(60)

and the discrete-vibrational-convective flux is determined by:
\[
R_{i+1/2,j} = |S|_{i+1/2,j} \left[ \begin{array}{c}
\rho_{a} \\
p_{a} \\
pav \\
pav \\
pavH \\
pavH \\
pato \\
pQ \end{array} \right] + \frac{1}{2} \left[ \begin{array}{c}
\rho_{a}^L \\
p_{a}^L \\
pav_{a}^L \\
pav_{a}^L \\
pavH_{a}^L \\
pavH_{a}^L \\
pato_{a}^L \\
pQ_{a}^L \end{array} \right] - \frac{1}{2} q_{i+1/2,j} \left[ \begin{array}{c}
\rho_{a}^R \\
p_{a}^R \\
pav_{a}^R \\
pav_{a}^R \\
pavH_{a}^R \\
pavH_{a}^R \\
pato_{a}^R \\
pQ_{a}^R \end{array} \right].
\]
(61)

The same definitions presented in [21-24] are valid to this algorithm. The time integration is performed employing the Euler backward method, first-order accurate in time, to the three types of convective flux. To the dynamic part, this method can be represented in general form by:
\[
Q_{i,j}^{(n+1)} = Q_{i,j}^{(n)} - \left(\Delta t_{i,j} / V_{i,j}\right) \times R\left(Q_{i,j}^{(n)}\right),
\]
(62)
to the chemical part, it can be represented in general form by:
\[
Q^{(n+1)}_{i,j} = Q^{(n)}_{i,j} - \Delta t_{i,j} \left[ R(Q^{(n)}_{i,j}) / V_{i,j} - S_{C}(Q^{(n)}_{i,j}) \right], \tag{63}
\]

where the chemical source term \(S_{C}\) is calculated with the temperature \(T_{mc}\) (reaction rate controlling temperature). Finally, to the vibrational part:

\[
Q^{(n+1)}_{i,j} = Q^{(n)}_{i,j} - \Delta t_{i,j} \left[ R(Q^{(n)}_{i,j}) / V_{i,j} - S_{v}(Q^{(n)}_{i,j}) \right], \tag{64}
\]

in which:

\[
S_{v} = \sum_{s=\text{mol}} q_{s-T-V} + \sum_{s=\text{mol}} S_{C,s} e_{v,s}, \tag{65}
\]

where \(q_{s-T-V}\) is the heat flux due to translational-vibrational relaxation, defined in [21-24].

The definition of the dissipation term \(\phi\) determines the particular formulation of the convective fluxes. The choice below corresponds to the [13] scheme, according to [31]:

\[
\phi_{i+1/2,j}^{nl} = \phi_{i-1/2,j}^{nl} = \begin{cases} 
M_{i+1/2,j}, & \text{if } |M_{i+1/2,j}| \geq 1; \\
0.5(M_{i+1/2,j} - 1)^{2}, & \text{if } 0 \leq |M_{i+1/2,j}| < 1; \\
0.5(M_{i+1/2,j} + 1)^{2}, & \text{if } -1 < M_{i+1/2,j} \leq 0.
\end{cases} \tag{66}
\]

This scheme is first-order accurate in space and time. The high-order spatial accuracy is obtained, in this study, by the ENO procedure.

The viscous formulation follows that of [32], which adopts the Green theorem to calculate primitive variable gradients. The viscous vectors are obtained by arithmetical average of the Green theorem to calculate primitive variable gradients. The viscous part corresponds to the first four equations of the Navier-Stokes ones plus the four equations of the turbulence model, the chemical part corresponds to the four equations immediately below the energy equation and the vibrational part corresponds to the equation below the last chemical species one.

### 6. ENO Procedure

ENO schemes overcome the limitations of TVD schemes by relaxing the requirement of total variation non-increasing:

\[
H_{0}([\xi_{i}]) = Q(\xi_{i}) = Q_{i}; H_{1}([\xi_{i}]) = Q(\xi_{i+1}) = Q_{i+1};
\]

\[
H_{00}([\xi_{i,j}]) = H_{1}([\xi_{i+1,j}]) - H_{0}([\xi_{i,j}]) / (\xi_{i+1,j} - \xi_{i,j}); \tag{68}
\]

\[
H_{000}([\xi_{i,j}, \xi_{i+1,j}, \xi_{i+2,j}]) = H_{01}([\xi_{i+1,j}, \xi_{i+2,j}]) - H_{00}([\xi_{i,j}, \xi_{i+1,j}]) / (\xi_{i+2,j} - \xi_{i,j}); \tag{69}
\]

If the divided difference \(H_{000}(\xi_{i,j}, \xi_{i+1,j}, \xi_{i+2,j})\) is larger than \(H_{00}(\xi_{i+1,j}, \xi_{i+2,j}, \xi_{i,3,j})\), choose \(H_{000} = H_{00}(\xi_{i+1,j}, \xi_{i+2,j}, \xi_{i,3,j})\); otherwise, \(H_{000}(\xi_{i,j}, \xi_{i+1,j}, \xi_{i+2,j})\) is accepted. This process is repeated until the required order of the interpolation is obtained and applied to each component of \(Q\) independently.

Note that the calculated stencil is computed dynamically at each point and is non-linear in nature. With the choice of the minimum divided difference at a point, the best molecule is determined to provide high accuracy.
After the determination of the coefficients of the Newton polynomial, the reconstruction process is finished:

\[\text{Rec}(\xi, Q) = Q(\xi_{i,j}) + H_0(\xi - \xi_{i,j}) + H_{i0}(\xi - \xi_{i,j}) + H_{0i}(\xi - \xi_{i,j}) + \ldots\]  

7. Turbulence Models

7.1. Coakley Turbulence Model

The [4] model is a \(k^{1/2}\)-\(\omega\) one. The turbulent Reynolds number is defined as

\[R = \sqrt{kN}/\nu_M.\]  

The production term of turbulent kinetic energy is given by

\[P = \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\frac{\partial u}{\partial y}/\text{Re}.\]  

\[P_k = \left(\frac{0.5C_1\nu}{\nu}\right)\frac{\omega\sqrt{k}/\text{Re}; D_k = 0.5 \left[2\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial x}\right)/\nu - 1\right]\frac{\omega\sqrt{k}/\text{Re}}{2/3\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial x}\right)/\nu}\right] \]  

where \(C_1 = 0.405D + 0.045\). The closure coefficients adopted for the [4] model are: \(\sigma_k = 1.0\); \(\sigma_\omega = 1.3\); \(C_\mu = 0.09\); \(C_2 = 0.92\); \(\beta = 0.5\); \(\alpha = 0.0065\); \(\text{Pr}_{DL} = 0.72\); \(\text{Pr}_{DT} = 0.9\).

7.2. Wilcox Turbulence Model

The turbulent viscosity is expressed in terms of \(k\) and \(\omega\) as:

\[\mu_T = \text{Re}^k k/\omega.\]  

In this model, the quantities \(\sigma_k\) and \(\sigma_\omega\) have the values \(1/\sigma^*\) and \(1/\sigma\), respectively, where \(\sigma^*\) and \(\sigma\) are model constants.

To the [5] model, the \(G_k\) and \(G_\omega\) terms have the following expressions:

\[G_k = -P_k + D_k\]  

\[G_\omega = -P_\omega + D_\omega,\]  

where:

\[\beta^* = 0.09; \beta = 3/40; \sigma^* = 0.5; \sigma = 0.5; \alpha = 5/9; \text{Pr}_{DL} = 0.72; \text{Pr}_{DT} = 0.9.\]

7.3. Yoder, Georgiadis, and Orkwis Turbulence Model

The turbulent Reynolds number is specified by:

\[\text{Re}_T = pk/\mu_M \omega.\]  

The parameter \(\alpha^*\) is given by:

\[\alpha^* = \alpha^* \left[1 + \text{Re}_T/R_k \right] \left[1 + \text{Re}_T/R_k \right].\]  

The turbulent viscosity is specified by:

\[\mu_T = \text{Re} \alpha^* pk / \omega.\]  

The source term denoted by \(G\) in the governing equation
contains the production and dissipation terms of $k$ and $\omega$. To the [6] model, the $G_k$ and $G_\omega$ terms have the following expressions:

$$G_k = -P_k + D_k \quad \text{and} \quad G_\omega = -P_\omega + D_\omega.$$  \hspace{1cm} (87)

To define the production and dissipation terms, it is necessary to define firstly some parameters. The turbulent Mach number is defined as:

$$M_T = \sqrt{2k/a^2}.$$  \hspace{1cm} (88)

It is also necessary to specify the function $F$:

$$F = \text{MAX}(M_T^2 - M_{T,0}^2, 0.0).$$  \hspace{1cm} (89)

The $\beta^*$ parameter is given by:

$$\beta^* = 0.09 \left[ 5/18 + (Re_T/Re_S)^4 \right] \left[ 1 + (Re_T/Re_S)^4 \right].$$  \hspace{1cm} (90)

Finally, the production and dissipation terms of Eq. (87) are given by

$$\mathcal{P}_k = \mu_T \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \frac{\partial u}{\partial y} ; D_k = \beta^* \rho \omega \left( 1 + \xi_k \right) F/Re ;$$  \hspace{1cm} (91)

$$\mathcal{P}_\omega = \alpha \omega / k P_k ; \quad \text{and} \quad D_\omega = \rho \omega^2 \left( 1 + \beta^* \omega^2 F \right)/Re ,$$  \hspace{1cm} (92)

with:

$$\alpha = 5/9 \left( \alpha_0 + Re_T / Re_S \right) \left( 1 + Re_T / Re_S \right) / \alpha^*.$$  \hspace{1cm} (93)

The [6] turbulence model adopts the following closure coefficients: $R_h = 8.0$, $R_k = 6.0$, $R_\omega = 2.7$, $\xi_k = 1.0$, $\xi_\omega = 0.0$, $\beta = 3/40$, $M_{T,0} = 0.0$, $\alpha_0 = 0.1$, $\alpha^*_0 = \beta^*/3$, $\sigma_k = 2.0$ and $\sigma_\omega = 2.0$.

### 8. Physical Problem and Mesh

![Figure 1. Blunt body viscous mesh.](image)

One physical problem is studied in this work: the blunt body problem. The geometry under study 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.

Figures 1 shows the viscous mesh used to the blunt body problem. This mesh is composed of 2,548 rectangular cells and 2,650 nodes, employing an exponential stretching of 5.0%. This mesh is equivalent in finite differences to a one of 53x50 points. A “O” type mesh is taken as the base to construct such mesh. No smoothing is used in this mesh generation process, being this one constructed in Cartesian coordinates.

### 9. Results

Tests were performed in a Core i7 processor of 2.1GHz and 8.0Gbytes of RAM microcomputer, in a Windows 8.0 environment. Four (4) orders of reduction of the maximum residual in the field were considered to obtain a converged solution; however, with the minimum of three (3) orders the author considered the solution converged. The residual was defined as the value of the discretized conservation equation. The entrance or attack angle was adopted equal to zero.

The initial conditions to this problem, for a five species chemical model, are presented in Tab. 1. To the seven species chemical model, the unique difference is the inclusion of $c_{NO^+}$ and $c_e$ with values equal to zero. $L_{REF}$ is the reference length, equal to L in the present study. The boundary conditions are described in [34]. The interested reader is encouraged to read this reference to become familiar with the present implementation. Reynolds number is obtained from [35].

### Table 1. Initial conditions to the problem of the blunt body.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_\infty$</td>
<td>8.78</td>
</tr>
<tr>
<td>$\rho_\infty$</td>
<td>0.0026 kg/m$^3$</td>
</tr>
<tr>
<td>$p_\infty$</td>
<td>687 Pa</td>
</tr>
<tr>
<td>$U_\infty$</td>
<td>4,776 m/s</td>
</tr>
<tr>
<td>$T_\infty$</td>
<td>694 K</td>
</tr>
<tr>
<td>$T_{wall}$</td>
<td>694 K</td>
</tr>
<tr>
<td>Altitude</td>
<td>40,000 m</td>
</tr>
<tr>
<td>$c_N$</td>
<td>$10^p$</td>
</tr>
<tr>
<td>$c_O$</td>
<td>0.07955</td>
</tr>
<tr>
<td>$c_{O_2}$</td>
<td>0.13400</td>
</tr>
<tr>
<td>$c_{NO}$</td>
<td>0.05090</td>
</tr>
<tr>
<td>$c_e$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>$c_{NO^+}$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>$L$</td>
<td>2.0 m</td>
</tr>
<tr>
<td>$Re_T$</td>
<td>2.3885x10$^5$</td>
</tr>
<tr>
<td>$k_0$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>$\omega_0$</td>
<td>$10\omega_{L_{REF}}$</td>
</tr>
<tr>
<td>$Q_h$</td>
<td>$10^{-3}$</td>
</tr>
</tbody>
</table>

#### 9.1. Coakley Results

5 Species Model. Figure 2 shows the pressure contours obtained by the [13] scheme as using the [4] turbulence model.
The value of the pressure peak is around 186.37 unities. Good symmetry properties are observed. The normal shock wave is well captured by the numerical algorithm.

Figure 2. Pressure contours (C).

Figure 3. Mach number contours (C).

Figure 3 exhibits the Mach number contours generated by the [13] numerical scheme as using the [4] turbulence model. Some pre-shock oscillations appear close to the oblique part of the shock wave. Although the Mach number peak is not significantly higher than the initial condition, it is suffice to generate pre-shock oscillations. Good symmetry properties are observed. The subsonic region behind the normal part of the shock wave is well captured.

Figure 4. Translational/rotational temperature contours (C).

Figure 4 presents the translational/rotational temperature contours obtained by the [13] numerical scheme as using the [4] turbulence model. A region of intense energy exchange is observed close to the body’s wall. The heat conduction along the body is well captured by the numerical scheme. Good symmetry properties are observed. The temperature peak is around 8,742.67 K, which agrees with standard values computed to this simulation (see [36]).

Figure 5. Vibrational temperature contours (C).

Figure 5 shows the vibrational temperature contours calculated by the [13] scheme as using the [4] turbulence model. Good symmetry properties are observed. The solution does not present pre-shock oscillations. The temperature peak is close to 1,772.23 K.

Figure 6. Turbulent kinetic energy contours (C).
Figure 6 exhibits the turbulent kinetic energy contours obtained by the [13] algorithm as using the [4] turbulence model. These contours show really the contours of $k^{1/2}$. The values are discrete. Good symmetry properties are observed. Figure 7 presents the vorticity contours obtained by the [13] scheme employing the [4] turbulence model. Good symmetry properties are observed. The vorticity values assume the expected ones for this problem. Figure 8 shows the $Q_s$ contours obtained by the [13] scheme employing the [4] turbulence model. Good symmetry properties are observed. The values of $Q_s$ are acceptable.

Figure 9 exhibits the $Q_s$ distribution around the blunt body, obtained by the [13] scheme as using the [4] turbulence model. Again good symmetry properties are observed. The range of values of $Q_s$ is acceptable.

Figure 10 presents the convergence history of this simulation. The convergence is reached in about 36,000 iterations. Several oscillations are present in the history due to the stiffness characteristic of the system of integral equations. Four (4) orders of reduction of the residual magnitude was reached.

As conclusion, the [4] turbulence model captures the main aspects of the flowfield to this problem. The convergence in more than 35,000 iterations to a reduction of 4 (four) orders of magnitude in the value of the residual is expected due to the reduced value of the CFL number (CFL $= 0.01$). However, the solution quality is excellent, even with the appearance of pre-shock oscillations in the Mach number contours.

7 Species Model. Figure 11 shows the pressure contours obtained by the [13] numerical scheme as using the [4] turbulence model. The stagnation pressure is higher than the theoretical value of 179.10 unities. Good symmetry properties are observed. The shock wave is well captured by the numerical scheme. Figure 12 exhibits the Mach number contours generated by the [13] scheme employing the [4] turbulence model. Pre-shock oscillations are observed close to the body upper surface. Reasonable symmetry properties are observed. The subsonic region close to the blunt body nose is well captured.
Figure 13 presents the translational/rotational temperature contours obtained by the [13] numerical scheme as using the [4] turbulence model. The temperature peak is close to the typical values obtained by this parameter in this study. Good symmetry properties are observed. The region of intense heat exchange due to conduction is formed close to the body wall, in the viscous layer. Figure 14 shows the vibrational temperature contours obtained by the [13] scheme employing the [4] turbulence model. The temperature peak is 1,771.38 K and is in accordance with typical values obtained in this work. Reasonable symmetry properties are observed.

Figure 15 exhibits the turbulent kinetic energy contours calculated with the [13] numerical scheme employing the [4] turbulence model. A low level of turbulence is observed from the legend. Good symmetry properties are observed. Figure 16 presents the vorticity contours calculated with the [13] numerical scheme as using the [4] turbulence model. A reasonable level of turbulence is observed. Good symmetry properties are again observed. Figure 17 shows the Q_h contours obtained by the [13] numerical scheme as using the [4] turbulence model.
Good symmetry properties are observed. The values of the $Q_h$ field are in accordance with the values of the other $Q_h$ ones, obtained by the other turbulence models. Figure 18 exhibits the $Q_s$ contours calculated with the [13] numerical scheme as using the [4] turbulence model. Good symmetry properties are observed. Typical values to $Q_s$ were obtained.

Figure 19 presents the convergence history obtained by the [13] numerical scheme as using the [4] turbulence model. Convergence in about 37,000 iterations is obtained. As explained above, this number of iterations is current in the CFD simulations to cases like this. The CFL number of 0.01 contributes to this occurrence.

9.2. Wilcox Results

Figure 20. Pressure contours (W).

Figure 21. Mach number contours (W).
5 Species Model. Figure 20 shows the pressure contours obtained by the [13] numerical scheme as using the [5] turbulence model. Good symmetry properties are observed. The stagnation pressure predicted by this turbulence model is closer to the theoretical value than the [4] one.

Figure 21 exhibits the Mach number contours generated by the [13] numerical algorithm as using the [5] turbulence model. The contours are free of pre-shock oscillations, although high values of Mach number were obtained. Good symmetry characteristics are observed. The subsonic region behind the normal shock portion of the shock wave is well captured.

Figure 22 presents the translational/rotational temperature contours obtained by the [13] numerical scheme employing the [5] turbulence model. The temperature peak is about 8,725.94 K. This value is in accordance with the average temperature field reached in the steady state. The viscous layer is well captured by the turbulence model. The region of high energy exchange due to heat conduction is well characterized in this figure. The shock wave is well captured by the numerical scheme.

Figure 23 shows the vibrational temperature contours obtained by the [13] scheme as using the [5] turbulence model. Good symmetry properties are observed. The vibrational temperature peak is also in accordance with previous results.

Figure 24 exhibits the turbulent kinetic energy contours obtained by the [13] numerical scheme as using the [5] turbulence model. A slightly unsymmetrical behavior is observed at the end of the body length. Values well above the respective ones obtained by the [4] model are observed, indicating that this solution presents more turbulent effects acting in the mean flow. Figure 25 presents the vorticity field obtained by the [13] algorithm employing the [5] turbulence model. More symmetrical aspects are observed in this case than in the turbulent kinetic energy case. This field is more intense than the respective one obtained with the [4] turbulence model.
Figure 26 shows the $Q_h$ contours obtained by the [13] scheme as using the [5] turbulence model. The solution is well developed and agrees with the respective solution obtained by the [4] model. Both fields present similar characteristics. Good symmetry properties are observed. Such solution assures that the boundary conditions were correctly stipulated. Figure 27 exhibits the $Q_s$ contours obtained by the [13] numerical algorithm as using the [5] turbulence model. Good symmetry properties are observed. The values obtained to this variable are in accordance with typical values expected to this parameter. Figure 28 presents the convergence history described by the [13] algorithm along its convergence to the steady state. Convergence in more than 45,500 iterations were observed to a reduction of 4 (four) orders in the residual magnitude. Stiffness characteristics are observed in the history.

7 Species Model. Figure 29 shows the pressure contours obtained by the [13] scheme employing the [5] turbulence model. Reasonable symmetry properties are observed. The stagnation pressure in this case is better than the last value obtained for it. Solution without pressure oscillations is observed. Figure 30 exhibits the Mach number contours obtained by the [13] scheme as using the [5] turbulence model. The solution presents pre-shock oscillation and instability free. Good symmetry properties and good capture of the subsonic region behind the normal portion of the shock are observed.

Figure 31 presents the translational/rotational temperature contours obtained by the [13] scheme as using [5] turbulence model. Good symmetry properties are observed. The heat conduction in the viscous layer is clearly captured. The temperature peak is in accordance with the peaks observed in the other turbulent solutions presented in this work. Figure 32 shows the vibrational temperature contours obtained by the [13] scheme as using the [5] turbulence model. Good symmetry properties are observed. The values of temperature are in agreement with the other vibrational temperature values observed in this study.

Figure 33 exhibits the turbulent kinetic energy contours obtained by the [13] numerical scheme as using the [5] turbulence model. The turbulent kinetic energy values are in fair agreement with the values obtained with the five species model to the same simulation. These values are higher than the respective ones obtained with the [4] turbulence model, indicating that more turbulence is present than indicated by the later. Reasonable symmetry properties are observed in both solutions, as in the five species as in the seven species.

Figure 34 presents the vorticity contours obtained by the [13] scheme as using the [5] turbulence model. Reasonable symmetry properties are observed. The level of vorticity is in agreement with the observed values in this study. Figure 35 shows the $Q_h$ contours obtained by the [13] scheme as using the [5] turbulence model. The peak of $Q_h$ indicates reasonable formation of static enthalpy fluctuations. The aspect of the $Q_h$ solution indicates that the boundary conditions were appropriated chosen. The five species solution is in close agreement with the seven species solution. Figure 36 exhibits the $Q_s$ contours generated by [13] as using the [5] turbulence model. Good symmetry properties are observed. The $Q_s$ field indicates that the fluctuation of mass fraction has occurred in the mean.
Figure 29. Pressure contours (W).

Figure 30. Mach number contours (W).

Figure 31. Translational/rotational temperature contours (W).

Figure 32. Vibrational temperature contours (W).

Figure 33. Turbulent kinetic energy contours (W).

Figure 34. Vorticity contours (W).
Figure 37. Convergence history (W).

Figure 37 presents the convergence history obtained by the [13] scheme employing the [5] turbulence model. Convergence in more than 46,000 iterations is observed. Stiffness problem is noted until 30,000 iterations. After 30,000 iterations, the convergence is smooth, without more oscillations.

9.3. Yoder, Georgiadids and Orkwis Results

5 Species Model. Figure 38 shows the pressure contours obtained by the [13] numerical scheme employing the [6] turbulence model. The stagnation pressure captured by the [13] scheme is the closest in relation to the theoretical value (179.10 unities). Good symmetry properties are observed, with slightly discrepancy at the body end.

Figure 38. Pressure contours (YGO).

Figure 39 exhibits the Mach number contours generated by the [13] numerical scheme as using the [6] turbulence model. A small pre-shock oscillation appears on the field but it is neglected in relation to the rest of homogeneous Mach number field. In spite of the high values of Mach number in the field, only this small oscillation has occurred, which indicates the good capacity of this ENO procedure in capture flows with normal shock waves and possibly other flow non-linear structures. Good symmetry characteristics are observed. The subsonic region behind the normal portion of the shock wave is well captured.

Figure 39. Mach number contours (YGO).
Figure 40. Translational/rotational temperature contours (YGO).

Figure 40 presents the translational/rotational temperature contours obtained by the [13] scheme as using the [6] turbulence model. The temperature field presents the average behavior of previous computations. The heat transfer is described by the conduction of heat along the body length. The viscous layer is also discerned by the region around the body, close to the wall.

Figure 41 shows the vibrational temperature contours generated by the [13] scheme as using the [6] turbulence model. Good symmetry aspects are observed. The temperature field presents typical behavior in relation with previous computations.

Figure 42 exhibits the turbulent kinetic energy contours generated by the [13] scheme as using the [6] turbulence model. Some asymmetrical aspects are observed in this figure. The kinetic energy peak is still above the value obtained with the [4] turbulence model. Figure 43 presents the vorticity contours obtained by the [13] algorithm employing the [6] turbulence model. These values are in common accord with the average values obtained in the present simulations. Although some asymmetrical aspects are present, its behavior is better than that of the turbulent kinetic energy variable.

Figure 44. $Q_h$ contours (YGO).

Figure 44 shows the $Q_h$ contours obtained by the [13]
numerical scheme employing the [6] turbulence model. Good symmetry properties are observed. The boundary conditions were correctly stipulated. The solution presents good homogeneous characteristics and the expected values. Figure 45 exhibits the Qs contours generated by the [13] algorithm as using the [6] turbulence model. Similarly to the Qh contours, the Qs contours present good homogenous features, good symmetry aspects and typical values to this variable. Again, the correct implementation of the boundary conditions was a remarkable aspect of these implementations.

Figure 45. Qs contours (YGO).

Figure 46 presents the convergence history described by the [13] scheme as using the [6] turbulence model. Oscillations due to stiffness problems are a remarkable aspect of this history. Convergence in more than 33,600 iterations to a reduction of 3 (three) orders of magnitude in the residual value was the characteristic of this history. Several oscillations are present in this history.

Figure 46. Convergence history (YGO).

7 Species Model. Figure 47 shows the pressure contours obtained by the [13] scheme as using the [6] turbulence model. Good symmetry properties are observed. The stagnation pressure is the closest of this model in relation to the theoretical value. Figure 48 exhibits the Mach number contours generated by the [13] scheme employing the [6] turbulence model. The solution is free of pre-shock oscillations, although high values of Mach number were obtained. Good symmetry features are noted. The subsonic region behind the shock wave is well captured by the scheme.

Figure 47. Pressure contours (YGO).

Figure 48. Mach number contours (YGO).

Figure 49 presents the translational/rotational temperature contours obtained by the [13] scheme employing the [6] turbulence model. Typical values are obtained by the temperature field. The viscous layer, defining a region of intense energy exchange and heat conduction, is well captured by the scheme. Good symmetry properties are observed. Figure 50 shows the vibrational temperature contours calculated with the [13] numerical algorithm and using the [6] turbulence model. Typical values of vibrational temperature
are also obtained in this simulation. Good symmetry properties are noted.

Figure 49. Translational/rotational temperature contours (YGO).

Figure 50. Vibrational temperature contours (YGO).

Figure 51. Turbulent kinetic energy contours (YGO).

Figure 52. Vorticity contours.

Figure 53. \(Q_h\) contours (YGO).

Figure 51 exhibits the turbulent kinetic energy contours generated by [13] employing [6]. Values intermediate between the [4] and the [5] models are obtained. Reasonable symmetry properties are observed. Figure 52 presents the vorticity contours generated by the [13] scheme as using the [6] turbulence model. Good symmetry properties are observed. The level of vorticity is in agreement with typical values of this study. Figure 53 shows the \(Q_h\) contours generated by the [13] scheme as using the [6] model. Good symmetry properties are noted. The range of values of static enthalpy fluctuation indicates that considerable turbulence is present. This turbulence is present in a moderate way in relation to the turbulent kinetic energy values.
Figure 54. \( Q_s \) contours (YGO).

Figure 55. Convergence history (YGO).

Figure 54 exhibits the \( Q_s \) contours calculated with the [13] algorithm as using the [6] model. Typical values of \( Q_s \) were obtained. Good symmetry properties are noted.

Figure 55 presents the convergence history of the [13] scheme as using the [6] turbulence model. The solution presents several oscillations with severe stiffness problems. The convergence occurs in three (3) orders of magnitude of the residual drop. Convergence in more than 33,600 iterations was observed.

9.4. Quantitative Analysis

In terms of quantitative results, the present authors compared the reactive results with the perfect gas solutions. The stagnation pressure at the blunt body nose was evaluated assuming the perfect gas formulation. Such parameter calculated at this way is not the best comparison, but in the absence of practical reactive results, this constitutes the best available result.

To calculate the stagnation pressure ahead of the blunt body, [37] presents in its B Appendix values of the normal shock wave properties ahead of the configuration. The ratio \( \frac{p_{r_0}}{p_{r_e}} \) is estimated as function of the normal Mach number and the stagnation pressure \( p_{r_0} \) can be determined from this parameter. Hence, to a freestream Mach number of 9.0 (close to 8.78), the ratio \( \frac{p_{r_0}}{p_{r_e}} \) assumes the value 104.8. The value of \( p_{r_e} \) is determined by the following expression:

\[
\frac{p_{r_e}}{\rho_{\infty}} = \frac{p_{r_0}}{\rho_{\infty} \times a^2_{\infty}}. \quad (94)
\]

In the present study, \( p_{r_0}^{\text{initial}} = 687\text{N/m}^2, \rho_{\infty} = 0.004\text{kg/m}^3 \) and \( a_{\infty} = 317.024\text{m/s} \). Considering these values, one concludes that \( p_{r_e} = 1.709 \) (non-dimensional). Using the ratio obtained from [37], the stagnation pressure ahead of the configuration nose is estimated as 179.10 unities. Table 2 compares the values obtained from the simulations with this theoretical parameter and presents the numerical percentage errors. As can be observed, the best turbulence model was [6], with an error of 2.859%. The best chemical model was the five (5) species chemical model, being slightly better than the seven (7) species chemical model as using the [4] turbulence model. It can be explained because in this problem the production of \( \text{NO}^+ \) and \( e^- \) was not high enough to highlight the seven (7) model as the best representation of the chemical field.

9.5. Computational Performance

Table 3 presents the computational data of the [13] scheme for the blunt body problem. It shows the CFL number and the number of iterations to convergence for all studied cases in the present work. As can be seen, the best performance is due to [13] when using the [4] turbulence model. Although the [6] turbulence model converges in less iterations, it is for three (3) orders of reduction of the residual magnitude. Hence, the [4] choice is the best for four (4) orders of reduction of the residual magnitude.

### Table 2. Values of stagnation pressure and errors.

<table>
<thead>
<tr>
<th>Turbulence Model</th>
<th>Chemical Model</th>
<th>( p_{r_0} )</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Seven Species</td>
<td>186.38</td>
<td>4.065</td>
</tr>
<tr>
<td>Wilcox [5]</td>
<td>Five Species</td>
<td>184.38</td>
<td>2.948</td>
</tr>
<tr>
<td></td>
<td>Seven Species</td>
<td>184.38</td>
<td>2.948</td>
</tr>
<tr>
<td></td>
<td>Seven Species</td>
<td>184.22</td>
<td>2.859</td>
</tr>
</tbody>
</table>

### Table 3. Computational data.

<table>
<thead>
<tr>
<th>Turbulence Model</th>
<th>Chemical Model</th>
<th>CFL</th>
<th>Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coakley [4]</td>
<td>Five Species</td>
<td>0.01</td>
<td>37,008</td>
</tr>
<tr>
<td></td>
<td>Seven Species</td>
<td>0.01</td>
<td>36,975</td>
</tr>
<tr>
<td>Wilcox [5]</td>
<td>Five Species</td>
<td>0.01</td>
<td>47,160</td>
</tr>
<tr>
<td></td>
<td>Seven Species</td>
<td>0.01</td>
<td>46,880</td>
</tr>
<tr>
<td>YGO [6]</td>
<td>Five Species</td>
<td>0.01</td>
<td>34,683</td>
</tr>
<tr>
<td></td>
<td>Seven Species</td>
<td>0.01</td>
<td>34,432</td>
</tr>
</tbody>
</table>
As final conclusion, it is possible to highlight the [6] turbulence model as the best in the estimative of the stagnation pressure ahead of the blunt body. The five species chemical model was more appropriate for this study in the absence of meaningful NO\(^{-}\) and e\(^{-}\) production. The [4] turbulence model was the most efficient in terms of computational performance. It is also important to note that all turbulence models predicted the stagnation pressure value with errors inferior to 5.000%.

10. Conclusion

In this work, a study involving the fourth-order ENO procedure using the Newton interpolation process from [9] is presented. The Favre averaged Navier-Stokes equations, in conservative and finite volume contexts, employing structured spatial discretization, are studied. The ENO procedure is presented to a conserved variable interpolation process, using the Newton method, to fourth-order of accuracy. Turbulence is taken into account considering the implementation of three k-\(\omega\) two-equation turbulence models, based on the works of [4-6]. The numerical algorithm of [13] is used to perform the reentry flow numerical experiments, which give us an original contribution to the CFD community. The “hot gas” hypersonic flow around a blunt body, in two-dimensions, is simulated. The convergence is accelerated to steady state condition through a spatially variable time step procedure [14-15]. The reactive simulations involve Earth atmosphere chemical models of five species and seventeen reactions, based on the [16] model, and seven species and eighteen reactions, based on the [17] model. N, O, N\(_2\), O\(_3\), and NO species in the former, whereas N, O, N\(_2\), O\(_3\), NO, NO\(^{-}\) and e\(^{-}\) species in the later, are used to perform the numerical comparisons.

As final conclusion, it is possible to highlight the [6] turbulence model as the best in the estimative of the stagnation pressure ahead of the blunt body. The five species chemical model was more appropriate for this study in the absence of meaningful NO\(^{-}\) and e\(^{-}\) production. The [4] turbulence model was the most efficient in terms of computational performance. It is also important to note that all turbulence models predicted the stagnation pressure value with errors inferior to 5.000%.

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References


