NUMERICAL EVALUATION OF THE FLOW INSIDE THE TRANSONIC NOZZLE OF A DIRECT-CONNECT SUPERSONIC COMBUSTION RESEARCH FACILITY

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Abstract. The direct-connect supersonic combustion research facility, now being assembled at the Combustion and Propulsion Laboratory (LCP/INPE) with the Institute for Advanced Studies (IEAv/CTA), consists basically of a vitiated air generator unit and a nozzle directly coupled to the supersonic combustor to be tested. The flow at the nozzle exit (i.e., at the combustor entrance) should simulate the conditions of the air behind the oblique or conical shock waves formed over the wedges, cones or other axisymmetric surfaces, used to compress the freestream in air breathing systems, such as scramjets (supersonic combustion ramjets) at hypersonic speeds. To simulate the same conditions of the air at the entrance of a scramjet combustor, in this ground test facility, oxygen enriched air is heated, by combustion of a fuel (hydrogen or hydrocarbon), inside a vitiated air generator (VAG) and then accelerated through the nozzle, thus feeding the combustor, under testing, with a “vitiated air” containing the desired air flow properties plus the combustion products generated in the heating process, while keeping the usual atmospheric oxygen content. To estimate the best relation between temperature test conditions at the nozzle exit and the fuel and oxidant mass flow rates in the injection plate, at the entrance of the VAG, the study of the flow inside the nozzle was needed. This paper shows the numerical evaluation of the transonic flow inside the convergent-divergent nozzle using the Jameson scheme, (which is a finite volume discretization method with artificial dissipative terms) for the solution of the Euler equations. The boundary conditions at the nozzle entrance are the stagnation conditions obtained in the combustion chamber of the VAG and at the nozzle exit are the conditions of the flow behind the oblique or conical shock waves formed ahead of wedges and cones under hypersonic speeds. For the marching in time it was used the Runge Kutta time-stepping scheme and equilibrium flow was assumed inside the nozzle. The specific heats ratios ($\gamma = c_p/c_v$) for the vitiated air and for the clean air are calculated and compared in order to evaluate the influence of the hydrocarbon traces on the test flow conditions.

Keywords: transonic nozzle, chemical reacting flow, supersonic combustion research facility

1. Introduction

The study of the supersonic combustion requires ground test facilities such as the scramjet direct-connect research facility (Dunsworth, 1979), now being assembled in the Combustion and Propulsion Laboratory (LCP/INPE) in Cachoeira Paulista. This facility consists basically of a vitiated air unit and a nozzle directly coupled to the supersonic combustor being tested, as shown in the schematic drawing in Fig. 1, and, at the nozzle exit, it should be generated, the same flow conditions of the air at a scramjet combustor entrance in actual flight. These conditions, at the combustor entrance, are the ones of the flow behind the oblique or conical shock waves formed ahead of the wedges or cone-noses of the vehicles flying at supersonic or hypersonic regimes.

The scheme of a scramjet combustor is shown in Fig. 2. The intake air (hypersonic flow) is slowed to supersonic speeds, by compression of the air against an oblique or conical surface in the entrance of the combustor (Heiser, 1994). The fuel is injected into the supersonic stream, where it mixes and burns in a combustion region downstream of the fuel injector strut. The expansion of hot gases through a supersonic nozzle at the back end of the engine, after fuel injection and combustion, accelerates the exhaust gas to a velocity higher than that of the inlet, generating thrust.

To simulate the same air conditions in the entrance of a scramjet combustor, in this ground test facility, oxygen enriched air is heated, by combustion, inside the vitiated air generator unit and then accelerated through a nozzle, thus feeding the combustor, under testing, with a “vitiated air” containing the desired flow properties, plus the combustion products, generated in the heating process, while keeping the desired atmospheric oxygen content (the presence of the combustion products in the air flow heating process, justifies its “vitiated air” label).
The main problem of this facility is finding the relation between the flow test conditions, at the nozzle exit, and the fuel and oxidizer (air plus $O_2$) mass flow rates in the fuel injection plate at the vitiated air generator (VAG). With the knowledge of this relation it is possible to control the desired tests conditions, changing only the oxidant and/or fuel mass flow(s). For this to be obtained it is necessary to evaluate the combustion process inside the VAG, to calculate the stagnation conditions at the nozzle entrance and to study the flow condition behind the oblique or conical shock waves to be simulated at the nozzle exit. These are the two boundary conditions needed to design the nozzle geometry that will yield the desired test conditions.

To obtain the boundary condition at the nozzle entrance a study was done to evaluate the combustion process inside the VAG, using the packages PSR and PLUG of the software CHEMKIN III, for benzene and hydrogen (Leite, 2003), where the combustion chamber was divided in two regions, i.e., two reactors: a perfectly stirred reactor (PSR) coupled to a plug flow one. This led to the estimating of the stagnation conditions (temperature and chemical composition) at the nozzle entrance. To obtain the conditions of the flow behind conical shock waves, a study was done for shock waves formed over the vertex of a circular cone with 15-degree semi angle under zero angle of attack flying at Mach numbers from 6 to 10 and altitudes ranging from sea level up to 80,000 m. To solve the governing equations it was developed an code using the software MATLAB 6.1, taking into account three gas models: the calorically perfect, the thermally perfect, and the equilibrium flow model (Leite, 2004) This led to the other boundary condition at the nozzle exit.

This work presents a study to adjust the test conditions, at the nozzle exit, and the fuel and oxidant (air + $O_2$) rates, at the VAG entrance. To analyze the flow inside the convergent-divergent nozzle, it was developed an algorithm with the software MATLAB 6.1, using the Jameson’s scheme, which is a finite volume discretization method with artificial dissipative terms, for the solution of the Euler equations. The specific heats ratios ($\gamma = c_p/c_v$) for the vitiated air and for the clean air are calculated, for temperature at the nozzle exit, and compared in order to evaluate the influence of the hydrocarbon traces on the test flow conditions.
2. Physical problem

To illustrate the physical problem to be solved, the schematic drawing of the vitiated air generator with the nozzle is shown in Fig. 3. The oxidant (air + O\textsubscript{2}) and the fuel QAV-1 (aviation kerosene) are injected in the combustion chamber of the VAG where they are mixed and burned. The kerosene QAV-1 is a mixture of various hydrocarbons and has the same composition as the kerosene for civil aircrafts engines Jet A-1 (or Jet A) and the JP-8, with an approximated global formula being C\textsubscript{11}H\textsubscript{21}. The QAV-1 composition varies from one batch to the other, so that, in order to develop a method for the nozzle flow calculation, it was assumed the fuel to be JP-10 because of its single-component hydrocarbon (C\textsubscript{10}H\textsubscript{16}) composition. This way it was made possible to obtain the detailed chemical mechanism (Li, 2001).

![Schematic drawing of the vitiated air generator with the nozzle.](image)

Using the method developed with the software CHEMKIN III\textsuperscript{®}, mentioned before, to evaluate the combustion process inside the VAG and considering the JP-10 chemical mechanism, it was obtained, for the initial mole fractions: \(J\)P-10 = 0.0127, \(O\textsubscript{2} = 0.3179\) and \(N\textsubscript{2} = 0.6694\), a combustion products mixing consisting of 35 different species, which mole fractions are shown in Table 1, and a stagnation temperature equal to 2299 K, at the combustion chamber exit. This can be considered the boundary condition at the nozzle entrance.

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N\textsubscript{2})</td>
<td>0.6397</td>
</tr>
<tr>
<td>(O\textsubscript{2})</td>
<td>0.1947</td>
</tr>
<tr>
<td>(CO_2)</td>
<td>0.6839E-01</td>
</tr>
<tr>
<td>(H_2O)</td>
<td>0.5447E-01</td>
</tr>
<tr>
<td>(CH_3)</td>
<td>0.1149E-01</td>
</tr>
<tr>
<td>(OH)</td>
<td>0.1125E-01</td>
</tr>
<tr>
<td>(CHO)</td>
<td>0.5094E-02</td>
</tr>
<tr>
<td>(O)</td>
<td>0.5018E-02</td>
</tr>
<tr>
<td>(CO)</td>
<td>0.4894E-02</td>
</tr>
<tr>
<td>(C_2H_6)</td>
<td>0.2387E-02</td>
</tr>
<tr>
<td>(NO)</td>
<td>0.1030E-02</td>
</tr>
<tr>
<td>(H_2)</td>
<td>0.5721E-03</td>
</tr>
</tbody>
</table>

At the nozzle exit it should be generated the conditions of the flow behind the oblique or conical shock waves formed ahead the wedges or nose-cones of the vehicles flying at hypersonic speeds, i.e., the conditions at the scramjet combustor entrance. In this work, it was considered the condition of temperature \((T_2)\) and Mach number \((M_2)\) of the flow behind an oblique shock wave formed over a wedge flying with the free stream Mach number \((M_\infty)\) equal to 7. This can be considered the boundary condition at the nozzle exit.
Figure 4 shows the relation between the temperature behind the shock \( T_2 \) and the free stream temperature \( T_\infty \) (Fig. 4a) and the Mach number (Fig. 4b), also behind the shock \( M_2 \), for a wedge with the angle ranging from 30 to 34 degrees, considering the calorically perfect gas model for the flow and the free stream Mach number equal to 7.

2.1. Governing equations

The following hypotheses are considered for the nozzle problem formulation: two-dimensional equilibrium flow, inviscid flow (where the dissipative transport phenomena of viscosity, mass diffusion, and thermal conductivity are neglected), there is no body force acting on the fluid and there is no heat addition.

The development of the following equations is detailed in Anderson (1995) and the main steps are described below.

The classical governing equations can be written in the conservation form as

Continuity equation (mass conservation equation)
\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0, \tag{1}
\]

Momentum equations
\[
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} + \frac{\partial (\rho uv)}{\partial y} = 0, \tag{2}
\]
\[
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho uv)}{\partial x} + \frac{\partial (\rho v^2 + p)}{\partial y} = 0, \tag{3}
\]

Energy equation
\[
\frac{\partial (\rho e)}{\partial t} + \frac{\partial[u(\rho e + p)]}{\partial x} + \frac{\partial[v(\rho e + p)]}{\partial y} = 0, \tag{4}
\]

where
\[
\varepsilon = e + \frac{1}{2}(u^2 + v^2) = \sum_{i=1}^{N} X_i e_i + \frac{1}{2}(u^2 + v^2) \tag{5}
\]
and
\[
e_i = h_i^0 + \int_{T_0}^{T} c_p dT - \frac{P}{\rho} \tag{6}
\]

In Eqs. (5) and (6), \( e \) is the internal energy per mass unit and \( X_i, e_i, c_p \) and \( h_i^0 \) are the mass fraction, the internal energy, the specific heat at constant pressure and the standard-state enthalpy for the \( i \)th species respectively. The velocity components in the \( x \) and \( y \) directions are defined as \( u \) and \( v \) respectively and \( t \) is the time.
Conservation of species equation
\[
\frac{\partial (\rho X_i)}{\partial t} + \frac{\partial (\rho u X_i)}{\partial x} + \frac{\partial (\rho v X_i)}{\partial y} = \omega_i W_i, \quad i = 1, \ldots, N.
\] (7)

Equation of state
\[
p = \rho R T \sum_{i=1}^{N} \frac{X_i}{W_i}.
\] (8)

In the above equations, \(\rho, p\) and \(T\) are the density, the static pressure and temperature, \(R\) is the universal gas constant, \(\omega_i\) and \(W_i\) are the net reaction rate and the specific weight of the \(i\)th species and \(N\) is the total number of species of the system.

2.2. Chemical reaction equations

The chemical mechanism of the fuel (JP-10) and the oxidant (air+O\(_2\)) includes 102 reactions with 28 irreversible ones (Li, 2001), and these reactions involve the 35 chemical species indicated in Table 1. Considering \(i\) as the indices of the species (with a total of \(N\)) and \(k\) as the indices of the reactions (with the total of \(K\)), the expression for the net production rate \(\dot{\omega}_i\), for the \(i\)th species can be written as
\[
\dot{\omega}_i = \sum_{k=1}^{K} V_{ik} q_k,
\] (9)

where \(V_{ik}\) is the stoichiometric coefficient (stoichiometric mole number) of the \(i\)th species and the \(k\)th reaction. The rate of progress variable \(q_k\) for the \(k\)th reaction is given by
\[
q_k = k_f \prod_{i=1}^{N} [C_i]^V_{ik} - k_b \prod_{i=1}^{N} [C_i]^{V^{-}_{ik}}.
\] (10)

where \([C_i]\) is the molar concentration of the \(i\)th species and \(k_f\) and \(k_b\) are the forward and backward rate constants of the \(k\)th reaction. The superscript ‘ indicates forward stoichiometric coefficients and " indicates backward stoichiometric coefficients.

The forward rate constant follows Arrhenius’s equation
\[
k_f = A_k T^\beta_k \exp \left( \frac{-Ea_k}{RT} \right),
\] (11)

where the pre-exponential factor \(A_k\), the temperature exponent \(\beta_k\), and the activation energy \(Ea_k\) are specified in the chemical reaction mechanism (Li, 2001). The backward rate constant \((k_b)\) is obtained from
\[
K_{ck} = \frac{k_f}{k_b},
\] (12)

where \(K_c\) is the concentration based equilibrium constant and it is related to the equilibrium constant based on partial pressures \(K_p\) by the following relation:
\[
K_{ck} = K_{pk} \left( \frac{P_{atm}}{RT} \right)^{\sum_{i=1}^{N} V_{ik}}
\] (13)

and \(K_{pk}\) can be found by the expression
\[
K_{pk} = \exp \left( \sum_{i=1}^{N} V_{ik} \frac{S_i}{R} - \sum_{i=1}^{N} V_{ik} \frac{H_i}{RT} \right)
\] (14)

where \(S_i\) is the entropy of the \(i\)th species.
The thermodynamic properties $C_p$, $H$ and $S$, were calculated assuming that they are thermally perfect, so that they are only functions of temperature, and may be given in terms of polynomial fittings (McBride, 2002).

The development of the complete set of equations is presented in Anderson (2000).

3. Numerical solution

The main objective of this work is to calculate the conditions of the flow, specially the temperature and the Mach number at the nozzle exit of the vitiated air generator (VAG). These will be the simulated conditions of the flow at the entrance of the scramjet combustor, under testing, at the supersonic combustion test facility, shown in Fig. 1. To obtain these data it was necessary to study the flow inside the convergent-divergent nozzle, considering the boundary conditions at the nozzle entrance to be the ones generated inside the combustion chamber of the VAG, given in Table 1, and, at the nozzle exit, the ones of the flow behind the oblique or conical shock waves generated ahead of the vehicles in hypersonic flight (Fig. 4).

One of the problems of this calculation is that the flow conditions at the combustion chamber exit, i.e., at the nozzle entrance, are the ones of the combustion products of the fuel (JP-10) and the oxidant (air + $O_2$), and this gas consists of a mixture of 35 species at 2299 K (Table 1). The recombination of these species, inside the nozzle, contributes to the final values of the temperature and of the Mach number at its exit, so that the chemical reactions have to be taken into account in the calculation. The idea of considering the 2-D Euler equations and the use of a CFD (Computational Fluid Dynamics) method to solve these equations, it is due to the fact that it is necessary to know the conditions of the entire flow field at the nozzle exit and not only at its centerline. This will help to know the values of the simulated flow conditions at the point where the fuels, which will be used for supersonic combustion studies, will be injected in the combuster under testing.

Numerical methods for solving Euler and Navier-Stokes equations have been developed since late sixties (MacCormack, 1969, 1982; Beam and Warming, 1978; Jameson, 1986; Mavriplis, 1988, 1990) and these methods are well known today. In Brazil there are groups such as the Centro Técnico Aeroespacial (CTA), in São José dos Campos, the Universidade Federal de Santa Catarina (UFSC) and the Pontifícia Universidade Católica (PUC), in Rio de Janeiro, that have been working on this subject for the past two decades. Also, many works in nozzle computations have been done during this period (Mason, 1980; MacCormack, 1997; Maciel, 2001).

To solve the 2-D governing Euler equations a code was developed in this work, with the software MATLAB 6.1®, using the Jameson’s scheme (Jameson, 1981), which is a finite volume spatial discretization method with artificial dissipative terms (Pulliam, 1986), because the Euler equations do not provide any natural dissipation mechanism, such as viscosity, in the Navier-Stokes equations, which would eliminate high frequencies caused by nonlinearities. The classical fourth order Runge-Kutta scheme was applied for the marching in time. The chemical reaction equations were solved simultaneously with the governing equations.

The Euler equations in the conservation form, i.e., Eqs. (1), (2), (3), (4) and (7), can also be written in the form:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \hat{\Omega} \quad (15)$$

where $Q$ (the solution or conserved quantities term), $E$ and $F$ (the flux terms) and $\hat{\Omega}$ (the source term) are interpreted as column vectors given by

$$Q = \begin{bmatrix} \rho u \\
\rho u^2 + p \\
\rho u v \\
u(2\rho e + p) \\
\rho X_{1u} \\
\rho X_{2u} \\
\cdots \\
\rho X_{N-1u} \end{bmatrix}, \quad E = \begin{bmatrix} \rho v \\
\rho u v \\
\rho v^2 + p \\
v(2\rho e + p) \\
\rho X_{1v} \\
\rho X_{2v} \\
\cdots \\
\rho X_{N-1v} \end{bmatrix}, \quad \hat{\Omega} = \begin{bmatrix} 0 \\
0 \\
0 \\
\dot{\omega} W_x \\
\dot{\omega} W_2 \\
\cdots \\
\dot{\omega} W_{N-1} \end{bmatrix}. \quad (16)$$

The mass fraction of the Nth species is calculated by
The system of equations is completed with the expressions for $p$ and $\varepsilon$ given by Eqs. (5) and (8).

The 2-D Euler equations for chemically reacting gas can also be written in integral form for Cartesian coordinates

$$\frac{\partial}{\partial t} \left( \int_{V} Q dx dy \right) + \int_{S} \left( Edy - Fdx \right) = \int_{V} Q dx dy$$

which for the $i$th control volume, assuming a stationary mesh, with the dissipative term becomes

$$\frac{d(Q_i)}{dt} = - \frac{1}{V_i} \left[ C(Q_i) - D(Q_i) \right] + \Omega_i(Q_i)$$

and where $C(Q_i), D(Q_i)$ and $\Omega_i(Q_i)$ are respectively the convective or flux, dissipative and source terms.

The code to solve Eq. (21) was developed using the software MATLAB 6.1. This software is a robust computational tool that allows solving the equations to analyze the physical phenomena under study (the Euler equations with the source term) using the algorithm chosen to solve them (Jamson’s method), where the software MATLAB® is used as the development tool. This approach of using the software MATLAB®, was interesting because all the other codes developed for the scramjet test facility, as the one to calculate the test conditions that should be generated at the nozzle exit (i.e., the flow conditions behind the shock waves), were developed with this same software. The data acquisition system of the facility is being developed using the software LabVIEW®, which is also a computational tool and is compatible with MATLAB®. This way, it will be possible to integrate all other systems of the supersonic combustion research facility, now being assembled, with the code developed in this work.

The problem was solved for a convergent-divergent nozzle with the following dimensions: throat radius = 10 mm, inlet radius = 30 mm, outlet radius = 20 mm and length = 80 mm, for a mesh of 40 cells in the $X$-axis and 20 cells in the $Y$-axis. The initial conditions were calculated with the software CHEMKIN-III®, for the combustion of the fuel (JP-10) and the oxidant (air+$O_2$) inside the VAG. The 1,500 mm long VAG’s combustion chamber (Fig. 3) was divided in two reactors: a perfectly stirred reactor (PSR), which is a small section located close to the fuel injection plate, and a plug flow reactor, coupled to the first one and using the two packages: AURORA/PSR and PLUG of CHEMKIN-III®, for the initial mole fractions of the reactants: $JP-10 = 0.0127$, $O_2 = 0.3179$ and $N_2 = 0.6694$, it was possible to obtain the stagnation conditions of the temperature and the mole fractions, at the end of the VAG’s combustion chamber. These are the combustion products conditions of those reactants mentioned above, which are used in the combustion process to heat up the air inside the VAG. The output of the code developed with the software CHEMKIN-III® (Table 1) is the initial condition (the input) for the nozzle code developed in this work. The boundary conditions at the nozzle exit are the ones calculated for the flow behind the shock waves and some of them are shown in Fig. 4.

Fig. 5 Temperature and Mach number distribution inside the nozzle. (nozzle centerline: $Y = 0$ mm)

The validation of the nozzle code developed here was done for the same nozzle geometry described above considering only the air with no chemical reactions, with the ratio of specific heats ($\gamma = c_p/c_v$) equal to 1.4. The results obtained were then compared with the tabulated data (Anderson, 1990) with a good agreement.
Figure 5 shows the values of temperature and Mach number distribution inside the nozzle, obtained with the developed nozzle code, for the boundary conditions specified above. This code, with two previous works: Leite (2003), where the combustion process inside the VAG was analyzed and Leite (2004), where the test condition that should be generated at the nozzle exit were calculated, completes the characterization of the entire flow field inside this supersonic combustion research facility.

Figure 6 shows the vitiated air temperature (a) and Mach number (b) distributions, along the Y-coordinate of the nozzle exit for the initial mole fractions of fuel and oxidizer (JP-10 = 0.0127, O$_2$ = 0.3179, N$_2$ = 0.6694) at the VAG’s entrance. The curves show that the flow conditions at the nozzle centerline (Y = 0) are approximately: temperature = 1225.0 K and Mach number = 2.2. Comparing these values with the ones obtained for the oblique shock wave formed ahead of a wedge flying at Mach 7 (Fig. 4) it is possible to see that considering, for example, an altitude equal to 70,000 m, where according to the Standard Atmosphere (NASA/ NOAA/ USAF, 1976) the free stream temperature ($T_\infty$) is 217.45 K, these conditions (for Y = 0) correspond to the ones for a deflection angle between 32 and 33 degrees.

With the variation of the fuel and/or the oxidizer mass flow rate, at the VAG entrance, it is possible to adjust the simulated values (Fig. 6), at the nozzle exit, with the desired conditions of the flow behind the oblique shock wave for the actual flight (Fig. 4). The vitiated air is composed by 35 species (Table 1), so the specific heats ratio ($\gamma = c_p/c_v$) of the vitiated air mixture is different from the one of the clean air (considering the four major component species: N$_2$, O$_2$, Ar and CO$_2$). To evaluate the influence of the hydrocarbon traces on the test flow conditions, the $\gamma$ values were calculated for the vitiated air, with the 35 species, and for the clean air, with the four major species mentioned before, considering the temperature distribution of Fig. 6a. These calculated values are displayed in Fig. 7.

The gamma ($\gamma$) values obtained for the vitiated air, for the case used as an example in this work, are very close to the ones obtained for the clean air at the same temperature (Fig. 7). This shows that the hydrocarbon traces generated by the combustion process in the VAG have low influence on the test flow conditions of the supersonic combustion research facility.
4. Conclusion

The main objective of this work is to evaluate the flow inside the transonic convergent-divergent nozzle of the supersonic combustion research facility which is being assembled in the LCP/INPE with IEAv/CTA assistance. The flow conditions at the nozzle exit, i.e., the conditions which should be generated by this ground test facility, are those of the flow behind the oblique or conical shock waves formed ahead of the noses of the vehicle in actual hypersonic flight. To obtain this result, oxygen enriched air is heated, by combustion, inside the vitiated air generator (VAG) unit and then accelerated through the nozzle. This study will help to design the nozzles geometry for the desired tests conditions and also it will help to find the relation between the flow test conditions and the mass flow rate of the fuel (JP-10/QAV-1) and the oxidant (air+O₂), for each experiment, at the VAG’s fuel injection plate.

The method developed in this work yields two main results. One is to possess the ability of adjusting the relation between the flow generated at the VAG nozzle exit and the ratio of the oxidant to fuel mass flow rates at the VAG’s unit entrance. The other is that it was shown that the specific heat ratio of the vitiated air generated (simulated) is almost the same of the clean air (the air without the traces of the combustion products) considering the same range of temperatures.

5. References