NUMERICAL EVALUATION OF THE COMBUSTION PROCESS IN A VITIATED AIR GENERATOR OF A DIRECT-CONNECTED SUPersonic COMBUSTION RESEARCH FACILITY

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Abstract. The direct-connected supersonic combustion research facility, now being assembled at the Combustion and Propulsion Laboratory (LCP) of the National Institute for Space Research (INPE) with the Institute for Advanced Studies (IEAv/CTA), consists basically of a vitiated air generator unit and a nozzle which is to be directly coupled to the supersonic combustor to be tested. The flow at the combustor inlet should simulate the conditions of the air behind the oblique or conical shock waves over wedges, cones or other axisymmetric surfaces used to compress the freestream flow in supersonic combustion air breathing systems like scramjets or ram accelerators. This is a high temperature, supersonic flow. The nozzle is designed to generate the desired Mach number and the air high temperature is obtained in the vitiated air generator by combustion. The evaluation of the combustion efficiency in the vitiated air generator shows the behavior of the fuel and air mass flow rates and the equivalence ratio needed to better control the stagnation temperature and the products composition. This control allows for the conditions achieved at the nozzle exit to be close to those of the air entering the combustor during actual flight operation, i.e., those of the air behind the oblique or conical shock waves formed at the entrance of scramjet engines or in front of the nose cone of ram accelerators in the super detonative mode. This paper discusses the combustion process in the vitiated air generator with fuels such as benzene ($C_6H_6$) and hydrogen ($H_2$) using the packages PSR and PLUG of the software CHEMKIN III.

Keywords: Supersonic Combustion, Hypersonic Flight, Scramjets, Ram Accelerators

1. Introduction

Supersonic combustion research requires ground test facilities such as shock tunnels, light gas guns (LGG) and supersonic combustion ramjet (scramjet) test benches (Dunsworth, 1979). Among these facilities the Institute for Advanced Studies (IEAv/CTA), in São José dos Campos has a shock tunnel and a LGG. The Combustion and Propulsion Laboratory (LCP/INPE), in Cachoeira Paulista is assembling a vitiated air generator facility for the testing of supersonic combustors and their components. The shock tunnel and the LGG units are versatile experimental ground test facilities, which operate for very short testing times. In these facilities the duration of the tests varies from microseconds to a few milliseconds, thus requiring specialized measurement techniques to obtain reliable pressure, velocity and temperature (heat flux) data. The scramjet combustor test facility, offers a testing time of about 10 seconds, which is appropriated for several experiments in supersonic combustion research activities.

The scramjet test facility, which is being assembled now, is a continuous flow direct-connected, as represented in the schematic drawing shown in Fig. (1), providing combustor inlet flow conditions corresponding to flight Mach numbers ranging from 5 to 7. The flow at the combustor entrance must simulate the conditions of the air behind the oblique or conical shock waves formed at the scramjet inlet engines or in front of the nose cone of ram accelerators operating in the super detonative mode.

Figure 1: Schematics of a direct-connected supersonic combustion test facility
As it is well known (Heiser, 1994), the air entering the intake of a scramjet is slowed, still to supersonic speeds, by compression of the air against an oblique or conical surface in the entrance of the combustor. Fuel (H\textsubscript{2} or a hydrocarbon) 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. The scheme of a scramjet combustor is shown in Fig. (2).

![Figure 2: Scramjet combustor scheme](image)

To simulate the same conditions of the air in the entrance of a scramjet combustor, in a ground test facility shown in Fig. (1), oxygen enriched air should be heated, by combustion, inside the vitiated air generator and then accelerated through the 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 fuels used in the vitiated air generator to heat the air are usually hydrogen or a hydrocarbon such as benzene or kerosene (JP-1, QAV-1). As the water vapor generated by the use of hydrogen may lead to ignition problems (Baranovskii, 1988), the facility assembled at LCP/INPE has been designed to operate with liquid hydrocarbon.

Since late fifties, experimental supersonic combustion research related to hypersonic air breathing propulsion has been actively taking place (Guy, 1996; Curran, 2001). The Combustion Heated Scramjet Test Facility (CHSTF) at NASA Langley Scramjet Test Complex (Andrews, 1985; Rogers, 1998), in operation since 1978, uses a vitiated-air test gas, which is obtained by hydrogen combustion. In Japan, the Vitiated-Heated Blowdown Tunnel of the Kakuda Research Center (Masuya, 1995; Boyce, 1998), vitiated-air is also obtained also by hydrogen combustion. Since 1995, the Air Force Research Laboratory Propulsion Directorate, Aerospace Propulsion Office (AFRL/PRA), has been developing a modern direct-connect test facility for full-scale scramjet combustor development (Gruber, 2001), with a cooling-water system, where available vitiated-air can be obtained by combustion of either liquid or gaseous fuel.

In order to control the combustion products and to better evaluate the desired temperature and the proper fuel to oxidizer (air plus O\textsubscript{2}) ratio, in the vitiated air generator, a study was done using the packages AURORA-PSR and PLUG, of the software CHEMKIN III, for benzene (C\textsubscript{6}H\textsubscript{6}) and hydrogen (H\textsubscript{2}), for comparison purposes. The temperature and species composition of the flow at the nozzle exit, has been compared with those of the air flow behind the oblique shock wave stabilized by a 15° wedge for upstream Mach numbers from 5 to 7, obtained with the package SHOCK of CHEMKIN III.

2. The vitiated air generator

The heart of the direct-connected scramjet combustor test facility is the vitiated air generator (VAG). It consists of an axisymmetric cylindrical chamber where the air is first enriched with oxygen and then heated by the combustion of a fuel, yielding the desired stagnation temperature before passing through a nozzle to be accelerated to the desired Mach number. Figure (3) shows the complete scheme of a VAG. The fuel injection plate and the enriched air diffuser are assembled in one side of the combustion chamber. On the other side there is a nozzle, which will be directly connected to the scramjet combustor to be tested. Early work in this field was done in Brazil during the nineties, dealing with a preliminary vitiated air generator with 200.00 mm of diameter and 900.00 mm long (Guimarães et al, 1993, 1996, jul/1997, dec/1997). This first
equipment allowed the evaluation of the efficiency of the whole system and the validation of design concept of the injection plate for liquid fuel.

The results obtained from the first system led to the construction of a second one, which has a larger diameter (310.00 mm), is longer (1,500.00 mm) and it is water cooled, as shown in Fig. (3), to assure the mechanical integrity of the material during longer and more frequent tests.

Figure 3: Schematics of the vitiated air generator

Figure (4) shows details of the new vitiated air generator. The picture on the left shows the injection plate, with eight swirlers, assembled on the support flange and the one on the right depicts the combustion chamber with the refrigeration channels around its external surface. Figure (5) shows the new VAG completely assembled.

Figure 4: Details of fabrication of the new vitiated air generator

Figure 5: The new vitiated air generator (VAG)
3. Flow conditions behind an oblique shock wave

The air conditions at the nozzle exit following the VAG combustion chamber should simulate the conditions of temperature and species composition of the air behind the oblique or conical shock waves over wedges, cones or other axisymmetric surfaces, used to compress the freestream flow in supersonic combustion air breathing systems. This is achieved by heating the air by combustion inside the VAG, and then accelerating it through the supersonic nozzle at the end of its combustion chamber as suggested in Fig. (3).

The purpose of this section is only to estimate the air temperature and species composition behind the shock wave to choose the best equivalence ratio and mass flow rates of fuel, O\textsubscript{2} and air for the combustion process used to heat the air inside the VAG.

To calculate the conditions behind the shock wave it was considered an oblique shock wave stabilized by a 15\degree wedge, with upstream Mach numbers of 5, 6 and 7, respectively, and it was used the package SHOCK of CHEMKIN III, because it yields both, the temperature and the species composition behind the shock, for a given upstream Mach number. The values of Mach numbers 5, 6 and 7 and the wedge angle of 15\degree used in the calculations were based on the conditions of the future experiments on supersonic combustion which will take place with the assistance of this VAG.

As the Application SHOCK of the CHEMKIN III collection calculates the conditions behind a normal shock, the value of the upstream Mach number used for the calculation was its normal component \(M_{n1}\).

The continuity equation for an oblique shock wave is (Anderson, 1990):

\[\rho_1 u_1 = \rho_2 u_2\]  

(1)

where \(\rho\) is the mass density.

The momentum equation applied to the oblique shock wave, represented in Fig. (6), and considering steady flow with no body forces (Anderson, 1990), yields:

\[(-\rho_1 u_1)w_1 + (\rho_2 u_2)w_2 = 0\]  

(2)

The geometric relation of an oblique shock wave over a wedge, shown in Fig. (6), can be expressed as:

\[M_{n1} = M_1 \sin \beta\]  

(3)
\[
\tan \beta = \frac{u_1}{w_1}
\]  

(4)

\[
\tan(\beta - \theta) = \frac{u_2}{w_2}
\]  

(5)

From the normal shock relations (Anderson, 1990 and Ames, 1953):

\[
\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M_{n1}^2}{(\gamma - 1)M_{n1}^2 + 2}
\]  

(6)

\[
\frac{p_2}{p_1} = 1 + \frac{2\gamma}{\gamma + 1}(M_{n1}^2 - 1)
\]  

(7)

\[
M_{n2}^2 = \frac{M_{n1}^2 + [2/(\gamma - 1)]}{[2\gamma/(\gamma - 1)]M_{n1}^2 - 1}
\]  

(8)

\[
\frac{T_2}{T_1} = \frac{p_2}{p_1} \frac{\rho_1}{\rho_2}
\]  

(9)

where \(T\) and \(p\) are respectively the temperature and pressure, and \(\gamma\) is the ratio of specific heats \(c_p/c_v\).

From Eqs. (1) to (6) it can be obtained:

\[
\frac{\tan(\beta - \theta)}{\tan \beta} = \frac{2 + (\gamma - 1)M_{n1}^2 \sin^2 \beta}{(\gamma + 1)M_{n1}^2 \sin^2 \beta}
\]  

(10)

Equation (10) can be expressed as:

\[
\tan \theta = 2 \cot \beta \left[ \frac{M_{n1}^2 \sin^2 \beta - 1}{M_{n1}^2 (\gamma + \cos 2\beta) + 2} \right]
\]  

(11)

Equation (11) is called the \(\theta-\beta-M\) relation, and specifies \(\theta\) as a function of \(M\), and \(\beta\). Graphical representation of this relation, for the cases of Mach numbers 5, 6 and 7 and \(\gamma = 1.4\), is shown in Fig (7).

Figure 7: Graphical representation of the \(\theta-\beta-M\) relation for Mach numbers 5, 6 and 7 (\(\gamma = 1.4\))
Equation (11) gives the value of $\beta$ correspondent to a specific given value of $\theta$ and to an upstream Mach number $M_1$. With the value of $M_1$ and $\beta$ it is possible to calculate the normal component of the upstream Mach number ($M_{n1}$) by Eq. (3) and with this we can have the conditions behind the shock wave from the normal shock relations given by Eqs. (6) to (9).

The normal component of $M_1$ ($M_{n1}$) is the input of the package SHOCK-CHEMKIN. Table (1) shows the values of $\beta$, $M_{n1}$, $M_{n2}$ and $M_2$, calculated for $\theta = 15^\circ$ and $\gamma = 1.4$, for Mach numbers 5, 6 and 7, using Eqs. (6) to (9).

Table 1: Values of $\beta$, $u_1$ and $M_{n1}$ calculated for $\theta = 15^\circ$ and $\gamma = 1.4$

<table>
<thead>
<tr>
<th>$M_1$</th>
<th>$\theta$</th>
<th>$\beta$</th>
<th>$u_1$ (m/s)</th>
<th>$M_{n1}$</th>
<th>$M_{n2}$</th>
<th>$M_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.00</td>
<td>15.00</td>
<td>24.3217</td>
<td>714.9649</td>
<td>2.0593</td>
<td>0.5676</td>
<td>3.5041</td>
</tr>
<tr>
<td>6.00</td>
<td>15.00</td>
<td>22.6719</td>
<td>802.9507</td>
<td>2.3127</td>
<td>0.5329</td>
<td>3.9918</td>
</tr>
<tr>
<td>7.00</td>
<td>15.00</td>
<td>21.5983</td>
<td>894.5938</td>
<td>2.5767</td>
<td>0.5059</td>
<td>4.4028</td>
</tr>
</tbody>
</table>

SHOCK is a CHEMKIN Application that predicts the chemical changes occurring after the shock heating of reactive gas mixtures or air dissociation. With the known conditions of the incident flow (upstream), such as velocity, pressure and temperature this package can calculate the flow conditions behind the shock wave (downstream) given by Eqs. (6) to (9) and also yields the mole fraction or concentration of each species due to chemical reaction or air dissociation.

As the Application SHOCK calculates the conditions of the flow behind a normal shock, the normal components of the velocity ($u_1$) and Mach number ($M_{n1}$), shown in Tab (1), were taken as inputs to this calculation. The upstream flow conditions of temperature and pressure considered for the three cases were: $p_i = 1$ atm and $T_i = 300$ K.

Table 2: Conditions behind the shock calculated by the application SHOCK-CHEMKIN III

<table>
<thead>
<tr>
<th>$M_1$</th>
<th>$p_1$ (atm)</th>
<th>$T_2$ (K)</th>
<th>$u_2$ (m/s)</th>
<th>$M_{n2}$</th>
<th>$O_2$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.00</td>
<td>4.7808</td>
<td>517.00</td>
<td>2577.5</td>
<td>0.5678</td>
<td>21.0</td>
</tr>
<tr>
<td>6.00</td>
<td>6.0808</td>
<td>581.30</td>
<td>2558.7</td>
<td>0.5328</td>
<td>21.0</td>
</tr>
<tr>
<td>7.00</td>
<td>7.5994</td>
<td>654.40</td>
<td>2567.9</td>
<td>0.5054</td>
<td>21.0</td>
</tr>
</tbody>
</table>

Table (2) shown the downstream flow conditions for the respective upstream Mach numbers ($M_1$). The velocity ($u_2$) and the Mach number ($M_{n2}$) are the respective normal components of the velocity and Mach number immediately behind the shock wave. Notice that for each one of the cases investigated here the temperature ($T_2$) behind the shock wave was always below 800 K so that dissociation does not take place. The $O_2$ mole fraction behind the shock remains 0.21 as desired.

The main purpose of this section was to estimate the temperature and species composition conditions for the air flow immediately behind an oblique or conical shock wave for a $15^\circ$ flow deflection angle for the three defined upstream Mach numbers. These should be the same conditions of the temperature and the $O_2$ composition for the vitiated-air at the exit of the supersonic nozzle (Fig. 3). With these conditions it is possible to calculate the stagnation conditions inside the VAG, at the end of the combustion chamber (Fig. 3). In section 4 it is shown the calculation of the stagnation conditions, the prediction of the $O_2$/air ratio in the oxidant and the best equivalence ratio for the fuel injection plate in the VAG.

4. Flow conditions inside the vitiated air generator

The present model assumes that the cylindrical 150.0 cm long combustion chamber can be divided in two regions, actually consisting in two reactors. One region, close to the fuel injection plate, can be considered a perfectly stirred reactor (PSR), where ignition takes place. The other region located immediately after the first one, can be considered a plug flow reactor (PFR), where the evolution of the conditions of the flow (temperature, velocity, pressure and species composition), along the reactor, can be studied.

After the air has been heated inside the vitiated air generator the flow passes through the nozzle to be accelerated to the Mach number ($M_2$), given in Tab. (1), and also to achieve the temperature ($T_2$), given in Tab. (2). From the isentropic relations for supersonic nozzle flow (Anderson, 1990 and Ames, 1953), we have:

$$\left(\frac{A_2}{A_1}\right)^2 = \frac{1}{M_2^2} \left[\frac{2}{\gamma + 1} \left(1 + \frac{\gamma - 1}{2} M_2^2\right)^\frac{\gamma + 1}{\gamma - 1}\right] \quad (12)$$

$$\frac{T_2}{T_o} = \left(1 + \frac{\gamma - 1}{2} M_2^2\right)^{-1} \quad (13)$$
\[
\frac{P_2}{p_o} = \left(1 + \frac{Z - 1}{2} M_2^2 \right)^\frac{-\gamma}{\gamma - 1}
\]

where \(A_2\) is the area at the exit of the nozzle, \(A^*\) is the cross section area of the throat, \(T_2\) and \(p_2\) are respectively the temperature and pressure at the exit of the nozzle.

\(T_o\) and \(p_o\) are the stagnation conditions of temperature and pressure inside the cylindrical chamber of the VAG, right before the throat of the divergent nozzle. Table (3) shows the values of \(T_o\) and \(A_2/A^*\) calculated, using Eqs. (12) and (13).

<table>
<thead>
<tr>
<th>(M_1)</th>
<th>(M_2)</th>
<th>(A_2/A^*)</th>
<th>(T_o/T_2)</th>
<th>(T_2) (K)</th>
<th>(T_o) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3.5</td>
<td>6.79</td>
<td>3.45</td>
<td>517.0</td>
<td>1783.65</td>
</tr>
<tr>
<td>6</td>
<td>4.0</td>
<td>10.72</td>
<td>4.20</td>
<td>581.3</td>
<td>2441.46</td>
</tr>
<tr>
<td>7</td>
<td>4.4</td>
<td>15.21</td>
<td>4.87</td>
<td>654.4</td>
<td>3186.93</td>
</tr>
</tbody>
</table>

In the present model it was considered a small reactor with 30.9 cm of diameter and 1.0 cm long where the oxygen, the air and the fuel are injected and mixed and where ignition takes place. In this reactor it was used the package AURORA-PSR of CHEMKIN III software to calculate the temperature and the flow species composition at the onset of ignition. This package assumes the reactor to be a perfectly stirred reactor (PSR) and it yields the species mole fractions and the temperature at its exit.

The conditions of species mole fraction and temperature of the first reactor (PSR) are the input values of the second reactor (PFR), which has the same diameter of the first one (30.9 cm) and it is 149.0 cm long. This second reactor is assumed to be a plug flow reactor, where one can study the development of the flow composition and temperature along the length of the reactor. Here it was used the package PLUG of the software CHEMKIN III. This way it was possible to evaluate the \(O_2/\text{air}\) ratio in the oxidant and the best equivalence ratio leading to the desired stagnation temperatures \(T_o\), shown in Tab. (3), while achieving the desired \(O_2\) mole fraction of 21% at the end of the second reactor.

This investigation dealt with two fuels: benzene (\(C_6H_6\)) as an example of a liquid hydrocarbon fuel and hydrogen (\(H_2\)), as an example of gaseous fuel. The kinetic mechanism used for the benzene-air mixture can be found in the work of Teodorczyk (1998). The residence times \(\tau\) used for the calculation with the PSR package were around: \(\tau = 0.14E-02\) seconds for \(H_2/O_2/\text{air}\) and \(\tau = 0.85E-03\) seconds for \(C_6H_6/O_2/\text{air}\).

The number of output or post-processor values obtained with the package PLUG is very large. Conditions such as temperature, velocity, residence time, species mole fractions, etc, can be plotted as a function of the distance (i.e., along the length of the reactor) or each one as a function of the other. For simplicity it is shown in Figs. (8) and (9) the curves of temperature and \(O_2\) mole fraction for different equivalence ratios of benzene and \(H_2\) relative to the reactor length \(X\).

In the case of benzene (\(C_6H_6\)), an oxidant mole composition consisting of 25% of air and 75% of \(O_2\) was kept while the equivalence ratio was changed from 0.5 to 0.8 (Fig. (8)). In the \(H_2\) case, the air to \(O_2\) ratio in the oxidant composition was changed while the equivalence ratio (ER) was kept constant, equal to 0.3 (Fig. (9)).
Figure 9: Flow conditions along the VAG for hydrogen, air and O₂ for different oxidant compositions

Figure (10) shows how the temperature and the O₂ mole fraction can be adjusted with a small change in the equivalence ratio. Notice that for the molar oxidant composition of 70% air and 30% O₂, a change in the equivalence ratio from 0.3 to 0.2 leads to the desired values of the temperature (\(T_o\)), given in Tab. (3) and to the desired O₂ mole fraction for Mach 5 flight test conditions.

Figure 10: Examples of temperature and mole fraction adjustments for different equivalence ratios

5. Conclusions

The direct-connect supersonic combustion ground test facility can be used for many different experiments where it is necessary to simulate the flow temperature, pressure and velocity behind the oblique or conical shock waves taking place over wedges and cones or other axisymmetric surfaces used to compress the freestream flow in supersonic combustion air breathing systems like scramjets or ram accelerators. This facility consists basically of a vitiated air generator unit (VAG), where O₂ enriched air is heated by combustion and accelerated through a nozzle to the Mach number needed for the experiment. The exit of the supersonic nozzle is to be directly coupled to the scramjet combustor to be tested. The air flow feeding the combustor under testing is 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 combustion process that was evaluated in this paper is the one occurring inside the combustion chamber of the VAG. The oxygen enriched air is heated, by combustion of a fuel which can be hydrogen or a hydrocarbon such as benzene or kerosene (JP-1, QAV-1). To estimate the best equivalence ratio and mass flow rates of fuel, O₂ and air for that combustion process, the vitiated air flow conditions behind the oblique or conical shock wave were predicted (section 3), so that those conditions should be the same at the exit of the supersonic nozzle. With these conditions, it was possible to calculate the stagnation conditions inside the VAG, at the entrance of the nozzle (section 4).
The packages AURORA-PSR and PLUG of the CHEMKIN III collection were used to find the best equivalence ratio and mass flow rates of fuel, O\textsubscript{2} and air for the combustion process inside the VAG to achieve the desired stagnation condition calculated in section 4.

The strategy of splitting the combustion chamber in two regions, one very short in length with a PSR (Perfectly Stirred Reactor) behavior and another one with a PFR (Plug Flow Reactor) behavior, which has been adopted in this work, seems to be satisfactory, although this will be confirmed later on through actual equipment testing. The results obtained from this study helped the design of the complex injection system of air, oxygen and fuel of the new supersonic combustion research test facility now being assembled at INPE. Is also important to notice that the tool developed in this work, using the software CHEMKIN III, will be very helpful in future scramjet combustor research activities.

Finally one should notice that obviously the conditions estimated across the oblique/conical shock waves were those of the vitiated air which will feed the supersonic combustor, prior to its arrival there, i.e., no supersonic combustion process is discussed here.

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7. References


