NUMERICAL EVALUATION OF THE FLOW INSIDE A SCRAMJET COMBUSTOR GROUND TEST FACILITY

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Abstract. *The studies of supersonic combustion require ground test benches such as the direct-connected supersonic combustion research facility, which is now being assembled at the Combustion and Propulsion Laboratory (LCP/INPE) with the assistance of the Institute for Advanced Studies (IEAv/CTA). This facility consists basically of a vitiated air generator (VAG) unit and a nozzle directly coupled to the supersonic combustor to be tested. The flow at the exit of the test facility simulates the air conditions behind the oblique or conical shock waves formed ahead of vehicles flying at hypersonic speeds. These are the same conditions at a scramjet (supersonic combustion ramjet) combustor entrance and it is a high temperature supersonic flow. To simulate this flow on the test facility, oxygen enriched air is heated by combustion inside the VAG and then accelerated through the nozzle, generating the "vitiated air" containing the desired flow properties plus the heating process combustion products, while keeping the same atmospheric oxygen content. In order to control and adjust the flow test conditions at the facility exhaust, an evaluation of the flow inside the entire facility should be done to find the relation between the test conditions at nozzle exit and the reactants (used to heat the air) mass flow rate at the VAG entrance. This work presents details of the study of the entire flow inside the facility where the combustion process in the vitiated air generator is analyzed, using the software CHEMKIN-III®, and the flow inside the nozzle is evaluated, using the Jameson scheme, which is a finite volume discretization method with artificial dissipative terms, for the solution of the Euler equations, considering three gas models: a calorically perfect, a frozen and a non-equilibrium one. This study allows us to adjust and control the test flow conditions, at nozzle exit, varying only the reactants flow rates, at the combustion chamber of the VAG entrance.*

Keywords*: supersonic combustion ground test facility, reactive flow, vitiated air generator, transonic nozzle.*

1. INTRODUCTION

The supersonic combustion ground test facility now being assembled, will be used specifically for testing scramjets combustors (Fig. 1), where the supersonic combustion occurs. To better understand how this facility works it is necessary to explain some characteristics of the scramjets and define the conditions of the flow behind the oblique or conical shock waves, which should be simulated in the facility. Scramjet engines are air-breathing propulsion systems which have no moving parts to compress the intake air, using instead the vehicles geometry to achieve the compression through the oblique or conical shock waves formed in front the noses of these vehicles flying at hypersonic speeds. Behind these shock waves the flow is still supersonic and has high temperature and these are the conditions of the air intake at the combustor entrance.

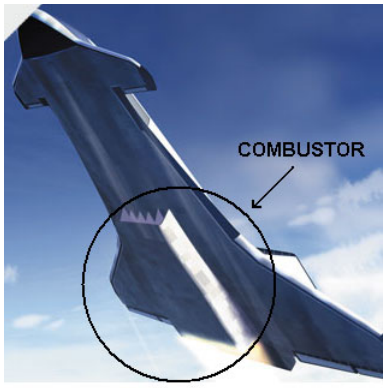


Figure 1: Illustration of a scramjet (Marshall, 2002) with the detail of the combustor.

Inside the combustor, the fuel (H_2 or a hydrocarbon) is injected into the supersonic stream, where it mixes and burns in a region downstream of the fuel injector strut (Fig. 2). The expansion of the 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.

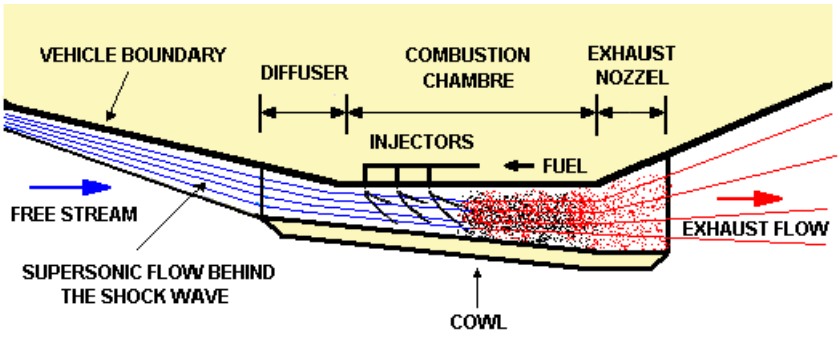


Figure 2: Schematic drawing of a scramjet engine (Curran, 1996).

The supersonic combustion ground test facility should generate the same conditions of the flow behind the oblique or conical shock waves formed during an actual flight and this flow will feed the combustor to be tested, as it is shown in Fig. 3. The complete facility consists basically of a vitiated air generator (VAG), where the flow is heated to the desired temperature, and a nozzle, where the heated air is accelerated to supersonic speeds, and with this it is possible to generate the flow test conditions. The combustor under testing is directly coupled to the nozzle exit, so because of that, this test facility it is called direct-connected.

To simulate in this ground test facility the same air conditions of the air at the entrance of a scramjet combustor in actual flight, 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 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 now being assembled at LCP/INPE was designed to operate with liquid hydrocarbon.

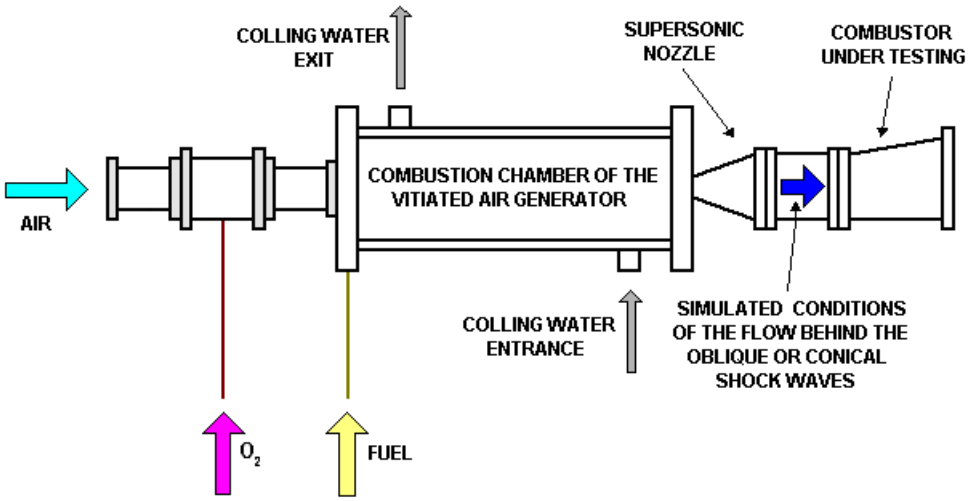
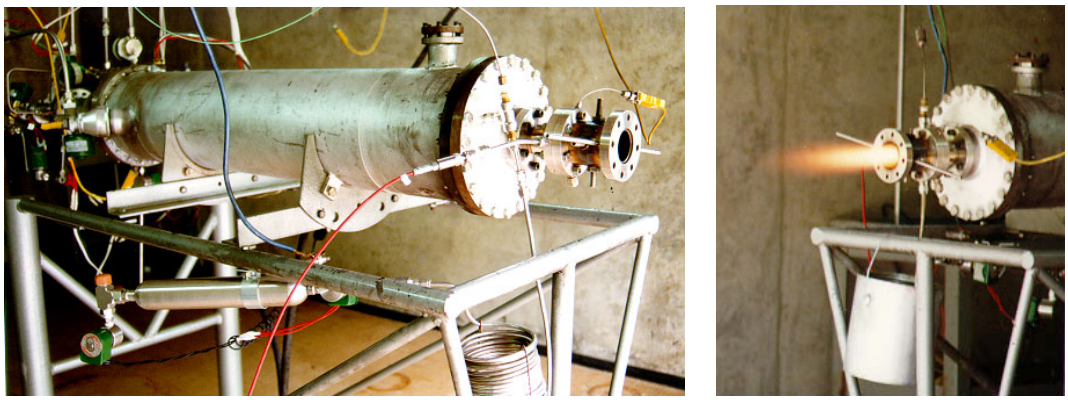


Figure 3: Schematic drawing of the direct-connect supersonic combustion test facility.

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 Brazil, early work in this field was done during the nineties, dealing with a preliminary vitiated air generator (Fig. 4a) with 200 mm of diameter and 900 mm long (Guimarães, 1996). 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. Figure 4b shows the detail of the supersonic heated flow at the nozzle exit, simulating the conditions behind the shock wave.



(a) (b)

Figure 4: The old vitiated air generator showing the supersonic heated flow at the nozzle exit (Guimarães, 1996).

The results obtained from the first system led to the construction of a second one, with a larger diameter (310 mm), longer (1,500 mm) and it is water cooled, as shown in Fig. 5, to assure the mechanical integrity of the material during more frequent and longer tests, which now have the duration around 20 s.

Figure 5: The new vitiated air generator (Leite, 2006).

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 at the vitiated air generator entrance. With the knowledge of this relation it is possible to control the desired tests conditions, changing only the reactants mass flow rates. To obtain this many other problems should be analyzed, such as for example: in the actual flight the conditions behind the shock waves are generated in the atmospheric air, so besides simulating the conditions of the temperature and Mach number, the vitiated air should have the same mole fraction of the air. The problem is that inside the VAG the air is heated by combustion and the oxygen is consumed in this process, so it is necessary enrich the air with O_2 at the VAG entrance to keep the desired oxygen mole fraction equal to 0.21 at the nozzle exit. The oxygen quantity that should be injected in the air is a parameter to be evaluated. A schematic drawing of the vitiated air generator with the fuel injection plate and the supersonic nozzle, is shown in Fig 6, where are indicated the conditions that should be controlled at the facility exit.

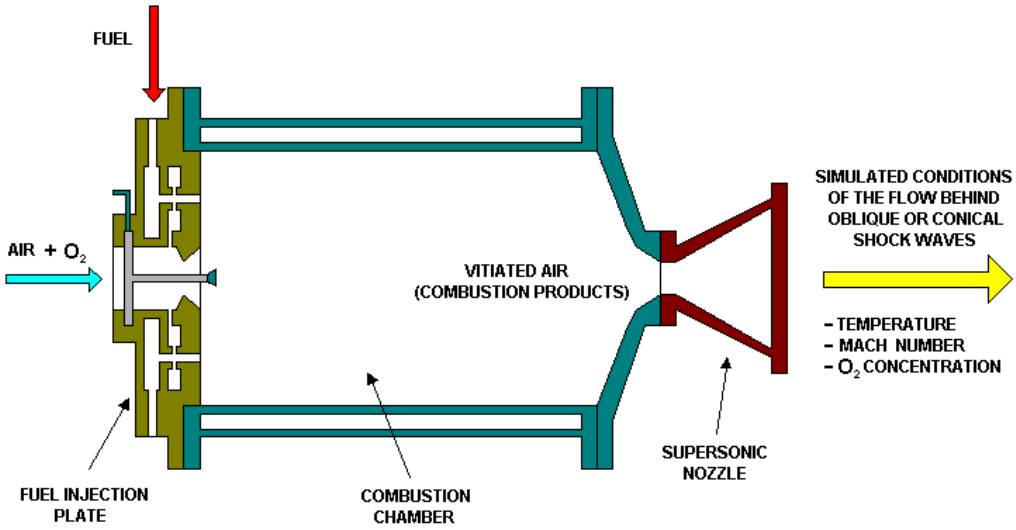


Figure 6: Schematic drawing of the vitiated air generator with the supersonic nozzle and flow conditions details.

Other problem is that the temperature inside the VAG can achieve values up to 3,000 K, so the O_2 can be dissociated and the vitiated air at the nozzle entrance, at stagnation conditions, can have a different chemical composition for each condition of pressure and temperature. Through the nozzle, the vitiated air is expanded and accelerated to supersonic speeds and with this expansion the temperature at the nozzle exit is around 1,000 K. So at the facility exit it can occur the vitiated air molecules recombination. The combustion process inside the VAG and the O_2 mole fraction after the recombination, at the facility exit, are also conditions that must be analyzed.

Another problem, related to the last one, is the chemical composition of the vitiated air at the nozzle exit, because the ratio of the specific heats ($\gamma = c_p/c_v$) of the vitiated air is different of the γ of the clean air, which is the air without the combustion products of the heating process, considering the same temperature at the nozzle exit. So, it is necessary to evaluate the influence of this difference between the two values of γ in the final results of the thermodynamics properties.

Besides all the problems mentioned before, there is the main one related to the global flow inside the entire facility. To this experimental apparatus really work as a ground test facility it is necessary to control the test flow conditions at the nozzle exit changing only the reactants flow rates at the VAG entrance. Because of this it became important to make the complete evaluation of the flow inside the facility to know all the phenomena involved in the process and with this obtain the relation between the flow conditions at the combustion chamber entrance of the vitiated air generator, which can be manipulated, and the test flow conditions at the nozzle exit, which should be simulated.

The complete characterization of flow inside the supersonic combustion research facility is divided, in this work, in two parts: the first is the evaluation of the combustion process inside the vitiated air generator to obtain the desired temperature condition at the combustion chamber exit and the second is the study of the flow inside the convergent-divergent supersonic nozzle to obtain the Mach number flow test conditions generated at the facility exit. The first part of the study was done using the software CHEMKIN-III® for the fuel JP-10 (Li, 2000; Purvis, 2001), in order to control the combustion products and to better evaluate the desired temperature and the proper fuel to oxidizer (air plus O_2) ratio, in the vitiated air generator. This first part of the study gives the stagnation conditions at the nozzle entrance. The second part is the evaluation of the flow inside the convergent-divergent supersonic nozzle. For this 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 γ for the vitiated air and for the clean air were calculated, for the same temperature distribution inside the nozzle, and compared in order to evaluate the influence of the hydrocarbon traces on the test flow conditions.

2. STUDY OF THE COMBUSTION PROCESS INSIDE THE VITIATED AIR GENERATOR

To evaluate the combustion process inside the VAG it was used a model in which the combustion chamber was divided in two reactors, as shown in Fig. 7. One, the region close to the fuel injection plate, can be considered a perfectly stirred reactor (PSR), where the ignition takes place. The other, located immediately after the first one, can be considered a plug flow reactor (PFR), where the evolution of the flow conditions (temperature, velocity, pressure and species composition), along the reactor, can be studied.

This strategy of dividing the combustion chamber in two regions was chosen because there are two different problems to be analyzed. One is where the fuel and oxidant mixture, the ignition and the combustion beginning occur, which was considered a PSR. In this model it is considered that the oxidant and the fuel are totally mixed, due to the

turbulence in the reactor region and because of this the conversion rate of the reactants in products is controlled only by the chemical reactions and not by the mixture process. The other region is where the combustion process finalization takes place was considered a PFR and is coupled to the first reactor, considering the approach of quasi-unidirectional flow. This model allows studying the evolution of the chemical composition of the reactive flow along the longitudinal axis of the reactor.

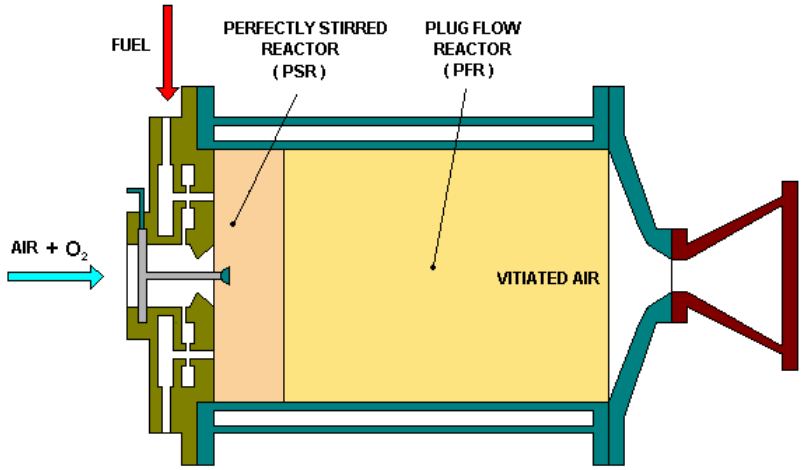


Figure 7: Schematic drawing of the VAG's combustion chamber division in two reactors.

The exit conditions of the first reactor (PSR) are the entrance conditions of the second one (PFR). To solve the problem, the package AURORA-PSR (Kee, 2000) was used to calculate the perfectly stirred reactor, and the package PLUG (Kee, 2000), was used for the plug flow reactor, both of the software CHEMKIN-III®.

2.1. Fuels used for the heating process of the air inside the VAG

For the heating process of the air inside vitiated air generators, the fuels usually used are the hydrogen (Boyce, 1998; Rogers, 1998) or hydrocarbon (Gruber, 2001). In the case of the facility which is being assembled will be used the liquid hydrocarbon QAV-1 (Petrobrás, 2000 and 2005), the aviation kerosene produced by Petrobrás. The QAV-1 is a mixture of many hydrocarbons and has their characteristics aligned with the kerosene Jet A-1 from AFQRJOS ("Aviation Fuel Quality Requirements for Jointly Operated System") and with the JP-8, used by USAF (United States Air Force), as shown in Petrobrás Specification (Petrobrás, 2005) and their global formula can be considered approximately as C11H21 (Cathonnet, 2003).

For the numerical evaluation of the VAG's combustion process, it was necessary to obtain the chemical kinetic mechanism of the oxidation of the fuel used in this process. For the QAV-1 this mechanism was not found, because each lot has a different composition and it is difficult to have a mechanism for each one, as the information given by Petrobrás. In the case of the Jet A, some woks were found but with only a few reaction and not for the complete mechanism (Degaut, 1994 and 2002). The same occurs with the JP-8 (Montgomery, 2002), where it is presented only a few reactions of the 573 ones, as mentioned in the work of Degaut (1994). As the kerosene QAV-1, the other two (Jet A and the JP-8) have also a different chemical composition for each lot.

Although it will be used the QAV-1 in the operation of the facility, for the numerical study of the flow conditions inside the VAG it was considered the kinetic mechanism of the JP-10 oxidation. The JP-10 ($C_{10}H_{16}$) is a single-component hydrocarbon, synthetically produced by hydrogenation of dicyclopentadiene, its reaction mechanism is given in reference Li (2001) and it was chosen because their characteristics are similar to the ones of the QAV-1. For comparison purposes, Tab. 1 shows the properties of the fuels: QAV-1, to be used in the ground test facility real operation, JP-10, used in the numerical calculations and the two others similar to the QAV-1 (Jet A and the JP-8).

Table 1: Comparison between the properties of the fuels: JP-10, QAV-1, Jet A and JP-8.

Fuel	Approximated Formula	Specific Energy (MJ/kg)	Density at 15°C (kg/m^3)
JP-10	$C_{10}H_{16}$	42.1	935.0
QAV-1	$C_{11}H_{21}$	42.8	804.0
Jet A	$C_{11}H_{21}$	43.4	799.0
JP-8	$C_{11}H_{21}$	43.2	809.0

The values shown in Tab. 1 were obtained from reference Purvis (2001) for JP-10, from the specifications Petrobrás (2000, 2005) for the QAV-1 and from Lewis (2001) for the Jet A and JP-8. Notice that the properties of these fuels indicated in Tab. 1 are very similar, especially the values of the specific energy.

As an illustration, Tab. 2 shows the 28 irreversible reactions (Li, 2000) of the 102 ones of the complete mechanism specific for the JP-10 ignition. The entire mechanism of the fuel JP-10 in CHEMKIN format is shown in Leite (2006). This mechanism was used for the calculation of the global flow conditions inside the VAG and the supersonic nozzle.

Table 2: Chemical kinetic mechanism for the JP-10 oxidation (Li, 2000).

k	Reactions	A	β	E_a
1	JP10+O2=>HO2+C3H5+C2H2+C5H8	7.920E13	0.00	47612.33
2	JP10+O2=>HO2+C3H3+C2H4+C5H8	3.980E13	0.00	50924.95
3	JP10+O=>OH+C3H3+C2H4+C5H8	2.880E06	2.40	5499.52
4	JP10+O=>OH+C3H5+C2H2+C5H8	2.760E05	2.60	1912.05
5	JP10+H=>H2+C3H3+C2H4+C5H8	1.320E06	2.54	6766.25
6	JP10+H=>H2+C3H5+C2H2+C5H8	2.600E06	2.40	4471.80
7	JP10+OH=>H2O+C3H5+C2H2+C5H8	3.800E06	2.00	-597.51
8	JP10+OH=>H2O+C3H3+C2H4+C5H8	1.740E07	1.80	980.40
9	JP10+HO2=>H2O2+C3H3+C2H4+C5H8	4.760E04	2.55	16508.13
10	JP10+HO2=>H2O2+C3H5+C2H2+C5H8	1.930E04	2.60	13907.74
11	JP10=>H+C3H3+C2H4+C5H8	6.000E16	0.00	98047.32
12	JP10=>H+C3H5+C2H2+C5H8	6.000E16	0.00	98135.76
13	JP10=>C2H2+2C2H4+C4H6	5.000E16	0.00	85444.55
14	C4H6=>C2H2+C2H3+H	1.580E16	0.00	109995.22
15	C4H6=>2C2H3	1.800E13	0.00	85126.67
16	2C2H3=>C4H6	1.260E13	0.00	0.00
17	C4H6+H=>C2H3+C2H4	5.000E11	0.00	0.00
18	C4H6+H=>H2+C2H2+C2H3	6.300E10	0.70	6001.43
19	C4H6+OH=>CHO+H+C3H5	5.000E12	0.00	0.00
20	C4H6+CH3=>CH4+C2H2+C2H3	7.000E13	0.00	18413.00
21	C3H3+CH3=>C4H6	5.000E12	0.00	0.00
22	C5H8=>C3H6+C2H2	1.000E16	0.00	72932.60
23	C5H8=>C3H4+C2H4	3.160E12	0.00	57074.57
24	C5H8=>C3H5+C2H3	3.160E12	0.00	57074.57
25	C5H8+O2=>C2H2+C3H5+HO2	3.000E12	0.00	0.00
26	C5H8+O2=>C2H3+C3H4+HO2	3.000E12	0.00	0.00
27	C5H8+HO2=>C2H2+C3H5+H2O2	1.000E14	0.00	0.00
28	C5H8+HO2=>C2H3+C3H4+H2O2	1.000E14	0.00	0.00

2.2. Numerical study of the flow conditions at the vitiated air generator exit using the fuel JP-10

To analyze the flow inside the VAG it is necessary to study the first reactor, the perfectly stirred reactor (PSR), exit conditions changes with the variation of the fuel and oxidant mass flow rate and the equivalence ratio ϕ between them, at the PSR entrance, considering various residence times τ and different oxidants compositions. A complete study of the combustion process inside the VAG is presented in reference Leite (2006), considering liquid hydrocarbons fuels (C_6H_6 and JP-10) and a gas (H_2). In the present work, the oxidant compositions considered were: 60% O_2 + 40% air, 70% O_2 + 30% air and 75% O_2 + 25% air. The volume defined for the PSR was 750 cm^3 and the area 750 cm^2 as the first reactor length is considered as 1 cm.

To use CHEMKIN III® to solve the problem it is necessary basically three files:

- The file with the code created by the user with the specific keywords of each package used (in the case of the present work they were the AURORA-PSR, for the PSR reactor and the PLUG for the plug flow one).
- The file with the chemical kinetic mechanism in CHEMKIN format, shown in Tab. 1.
- The file with the thermodynamic data in CHEMKIN format, shown in Tab 3 for the species JP-10 and N_2, as an exemple.

Table 3: Example of the thermodynamic data file for JP-10 e N_2 in CHEMKIN III® format.

```
JP10                    C  10H  16O   00   0G  300.00   5000.00     1000.00    1
-4.78290200E+00 9.08977000E-02-4.73497000E-05 9.36283900E-09-3.17350600E-12    2
-9.13640100E+03-1.59228000E+01-4.78290200E+00 9.08977000E-02-4.73497000E-05    3
 9.36283900E-09-3.17350600E-12-9.13640100E+03-1.59228000E+01                   4

N2                121286N   2             G0 300.00   5000.00    1000.00      1
 0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13    2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-0.03963222E-04    3
 0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02                   4
```

The thermodynamic data table gives, in lines 2, 3 and 4 the coefficients from A_1 to A_7 used in Eqs. (1), (2) and (3) for each species *i* involved in the mechanism and theses values can be obtained in McBride (1963).

$$\frac{C_{pi}^o}{\Re} = A_{1i} + A_{2i}T_i + A_{3i}T_i^2 + A_{4i}T_i^3 + A_{5i}T_i^4 \tag{1}$$

$$\frac{H_i^o}{\Re T_i} = A_{1i} + \frac{A_{2i}}{2}T_i + \frac{A_{3i}}{3}T_i^2 + \frac{A_{4i}}{4}T_i^3 + \frac{A_{5i}}{5}T_i^4 + \frac{A_{6i}}{6} \tag{2}$$

$$\frac{S_i^o}{\Re} = A_{1i}\ln T_i + A_{2i}T_i + \frac{A_{3i}}{2}T_i^2 + \frac{A_{4i}}{3}T_i^3 + \frac{A_{5i}}{4}T_i^4 + A_{7i}\,. \tag{3}$$

The 80 columns of the four lines of Tab. 3 are divided in 5 blocks of 16 columns each, which the five blocks of line 2 and two blocks on the left of line 3 give the coefficients A_1 to A_7 for low temperatures and the three blocks on the right of line 3 and the four block of line 4 give the coefficients A_1 to A_7 for high temperatures. With these coefficients the properties C_{pi}^o, H_i^o and S_i^o can be calculated and with these properties and the values of the pre exponential factor *A*, the temperature coefficient β and activation energy E_a, (Tab. 2) it is possible to solve all the equations necessary to obtain the solution of the flow inside the VAG. The complete development of these equations is shown in Leite (2006).

For the three cases studied (the three different oxidant compositions) the residence time was considered to be equal to τ = 2E-2 s. Table 4 shows the exit flow conditions of the perfectly stirred reactor (PSR) for these three cases.

Table 4: PSR exit flow conditions = PFR entrance conditions for the fuel JP-10.

Oxidant Composition	τ (s)	ϕ	$T_{exit\ PSR}$ (K)	$MF_{exit\ PSR}\ O_2$	$\dot{m}_{exit\ PSR}$ (g/s)
60% O_2 + 40% air	2E-2	0.84	1877	0.1920	183
70% O_2 + 30% air	2E-2	0.73	2256	0.2141	153
75% O_2 + 25% air	2E-2	0.675	2667.2	0.1963	130

These conditions (Tab. 4) are considered as the entrance conditions for the calculation of the second reactor, the plug flow reactor (PFR). The resume of the PFR exit flow conditions is shown in Tab. 5, where the temperature $T_{exit\ PFR}$ and the mole fraction $MF_{exit\ PFR}$, which were calculated with the package PLUG of the CHEMKIN III® software, are given at the VAG exit (longitudinal axis *x* = 150 cm). The pressure inside the VAG was considered equal to 25 atm.

Table 5: PFR exit conditions = stagnation conditions at the entrance nozzle for the fuel JP-10.

Oxidant Composition	ϕ	$T_{exit\ PFR}$ (K)	$MF_{exit\ PFR}\ O_2$
60% O_2 + 40% air	0.84	1938.0	0.1838
70% O_2 + 30% air	0.73	2247.2	0.2109
75% O_2 + 25% air	0.675	2667.2	0.1960

Table 5 shows, in the fourth column, only the value of the oxygen mole fraction because this is a parameter that has to be controlled, but for the study of the flow inside the supersonic nozzle, which is presented in the next section, all the others species of the vitiated air must be considered. So choosing the case where the oxidant is composed by 75% O_2 + 25% air and the fuel/oxidant equivalence ratio is equal to 0.675 the value of the mole fraction for all the vitiated air species is given in Tab 6.

Table 6: Mole fraction of the vitiated air species for the case 75% O_2 + 25% air and ϕ = 0,675 at the VAG exit.

JP-10 = 8.160E-92	C_5H_8 = 4.019E-94	C_4H_2 = 4.802E-27
C_4H_3 = 2.948E-42	C_4H_6 = 9.062E-43	C_3H_3 = 1.948E-28
C_3H_4 = 2.200E-31	C_3H_5 = 7.510E-03	C_3H_6 = 4.504E-03
C_2H = 5.963E-23	C_2H_2 = 4.695E-21	C_2H_3 = 1.221E-25
C_2H_4 = 3.564E-26	C_2HO =-2.206E-21	CH = 1.258E-16
CH_2 = 1.454E-16	CH_3 = 1.995E-16	CH_4 = 2.408E-17
CHO = 5.145E-03	CH_2O = 7.608E-11	CH_3O = 2.005E-17
H = 2.806E-04	H_2 = 7.920E-04	H_2O = 1.378E-01
H_2O_2 = 3.158E-06	HCO = 5.247E-09	HO_2 = 5.472E-05
O = 2.754E-03	O_2 = 1.960E-01	OH = 1.237E-02
CO = 6.654E-03	CO_2 = 1.770E-01	N = 1.621E-07
N_2 = 4.274E-01	NO = 2.175E-02	

The values shown in Tab. 5 and 6 are the boundary conditions at the supersonic nozzle entrance, used for the study of the flow inside the nozzle to be presented in Section 3.

3 EVALUATION OF THE FLOW INSIDE THE SUPERSONIC NOZZLE

The study of the flow conditions inside the convergent-divergent supersonic nozzle of the facility (Fig. 6) was done specially to create a tool that allows calculating the test conditions at the nozzle exit of the facility. For this study it was used the geometry of the nozzle, which was coupled to the old VAG (Fig. 4), to know which test conditions it is possible to obtain using this nozzle with the new VAG (Fig. 5). As the mole fraction of the O_2 is also a parameter that should be controlled and must be equal to 0.21, in this study it was considered the chemical reactions of recombination that occurs during the expansion process inside the divergent part of the nozzle. So for comparison purposes the study was done for three gas models: the calorically perfect, in which the γ value is considered to be equal to 1.4, the frozen model, where the γ value is calculated considering the temperature and the mole fraction of the species at the stagnation condition and this value is considered constant along the nozzle and the third model, the non-equilibrium one, in which the chemical reaction are taken into account.

To analyze the flow inside the nozzle it was developed a code with the software MATLAB 6.1® to solve the Euler equations 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.

3.1. Governing and chemical reaction equations

The following hypotheses are considered for the nozzle problem formulation: two-dimensional 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 governing equations is detailed in Anderson (1995) and the chemical equations describing the reactive flow are presented in Anderson (2000). The classical governing equations, i.e., continuity, momentum, energy, species conservation and the equation of state are then solved along with the chemical reaction equations using the chemical kinetic mechanism of the fuel (JP-10) with the composed oxidant (air + O_2) including 102 reactions with 28 irreversible ones (Li, 2001). To obtain the solution of the chemical reaction equations it is necessary to calculate the properties C_{pi}^o, H_i^o and S_i^o, by Eqs. (1), (2) and (3) for each species *i* involved in the mechanism. The development of the complete set of equations to solve the problem is present in Leite (2006).

3.2. Numerical solution

This problem was then solved numerically for the three gas models mentioned above, considering a nozzle with the following dimensions: throat radius = 10 mm, inlet radius = 30 mm, outlet radius = 20 mm and length = 80 mm, for a structured mesh with 100 cells in the X-axis and 20 cells in the Y-axis. To illustrate the results of this calculation Fig. 8 shows the temperature and Mach number distributions along the nozzle and Fig. 9 displays the O_2 mole fraction distribution obtained for the non-equilibrium gas model.

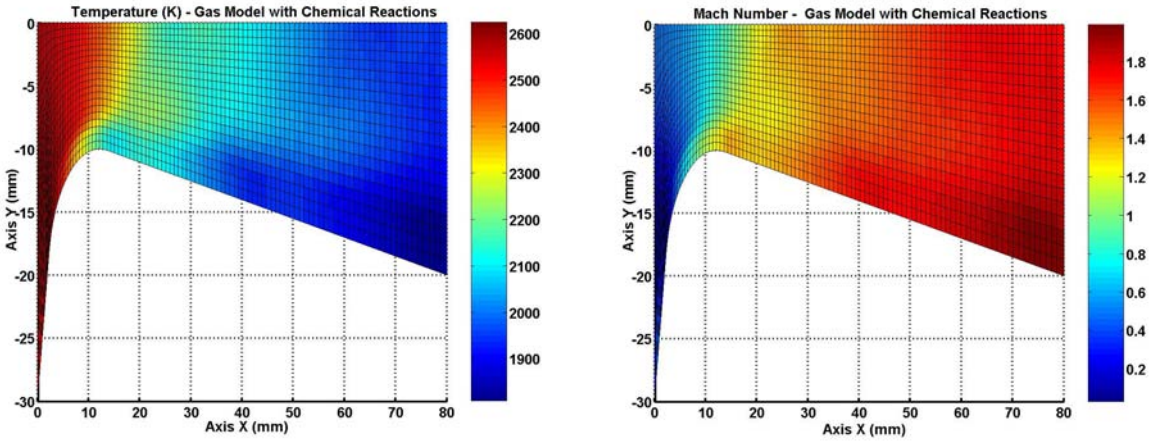


Figure 8: Temperature and Mach number distributions along the nozzle for the non-equilibrium gas model

In this calculation it was considered a stagnation pressure and temperature of 25 atm and 2667.2 K (Tab. 5) respectively and the mole fraction of the vitiated air species, shown in Tab. 6. Notice in Fig. 9 that the value of the O_2 mole fraction is 0.196 at the nozzle entrance and 0.208 at its exit. With the expansion of the gas inside the nozzle the O_2 mole fraction is higher at its exit due to the molecules recombination (Fig. 9).

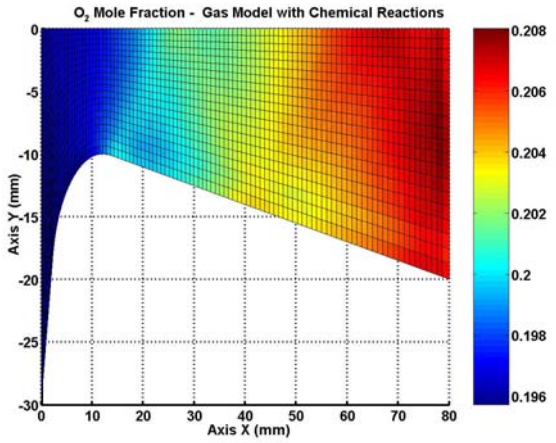


Figure 9: O_2 mole fraction distribution along the nozzle for the non-equilibrium gas model.

The same calculation was done also for other two gas models, the calorically perfect and frozen, considering the same stagnation conditions used for the non-equilibrium model. For the calorically perfect gas γ was considered constant along the nozzle and equal to 1.4 and for the frozen gas model γ was calculated for the conditions shown in Tables.5 and 6. So that $\gamma = 1.2213$ and this value was kept constant along the nozzle. For comparison purposes Fig. 10 shows the temperature and the Mach number along the nozzle centerline for the three gas models. These values were calculated for the initial conditions, at the VAG's combustion chamber entrance, shown in Tab. 5 (oxidant composition = 75% O_2 + 25% air and $\phi = 0.675$) and with this calculation it was obtained the desired relation between the flow conditions at facility entrance (fuel and oxidant mass flow rate) and the flow test conditions generated at the facility exit, which simulates the flow behind the oblique or conical shock waves (Anderson, 1990).

As an example, considering the values obtained for the frozen gas model in Fig. 10 at the nozzle exit (X = 80 mm), the value of temperature is around 2000 K and Mach number 1.8, and these are the conditions of the flow behind the oblique shock wave formed in front of a vehicle with the shape of a wedge with 35° flying with Mach 8 speed.

The curves shown in Fig. 10 represent the values of temperature and Mach number along the nozzle centerline for the three gas models considered in this work. Notice that for the model where the chemical reactions were taken into account, the temperature at the nozzle exit is higher than the ones for the other models. This is so because the molecules recombination is an exothermic process.

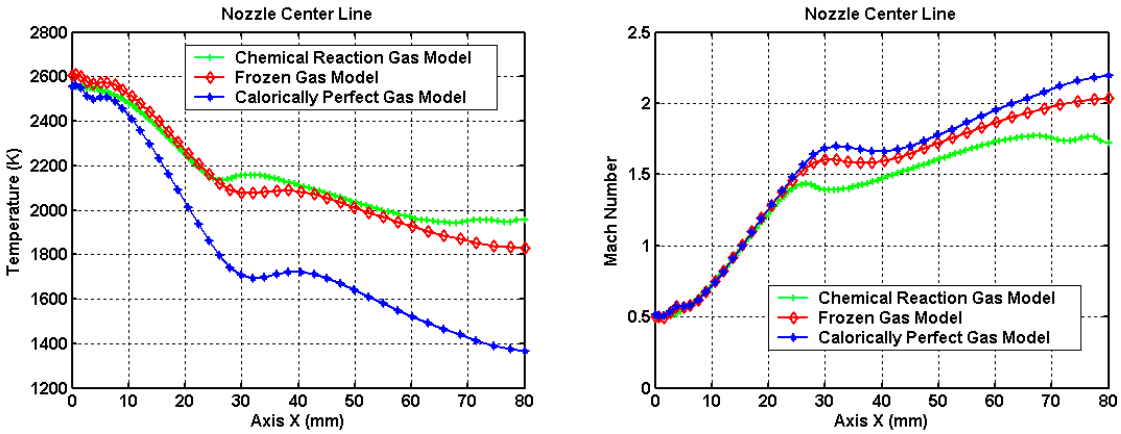


Figure 10: Comparison between the values of temperature and Mach number for the three gas models.

Another important evaluation is the comparison between the values of γ for the vitiated air and the clean air. This led to the calculation of the dissociated clean air mole fraction, under the same stagnation conditions of the vitiated air (T = 2667.2 K and p = 25 atm), shown in Tab. 7, to be used as boundary conditions for the clean air case.

Table 7: Mole fraction of the clean air for T = 2667.2 K and p = 25 atm.

Ar = 0.00959	N = 2.17E-07	NO_2 = 9.78E-05
O_2 = 0.19280	NO = 0.02992	N_2 = 0.76486
O = 2.73E-03	N_2O = 7.41E-06	

Figure 11 shows the values of γ for the vitiated and the clean air, along the nozzle, calculated for the same temperature distribution shown in Fig. 8. As the difference between the two values is around 4% the traces of existent hydrocarbons in the vitiated air have no influence on the flow properties calculated for the vitiated air case.

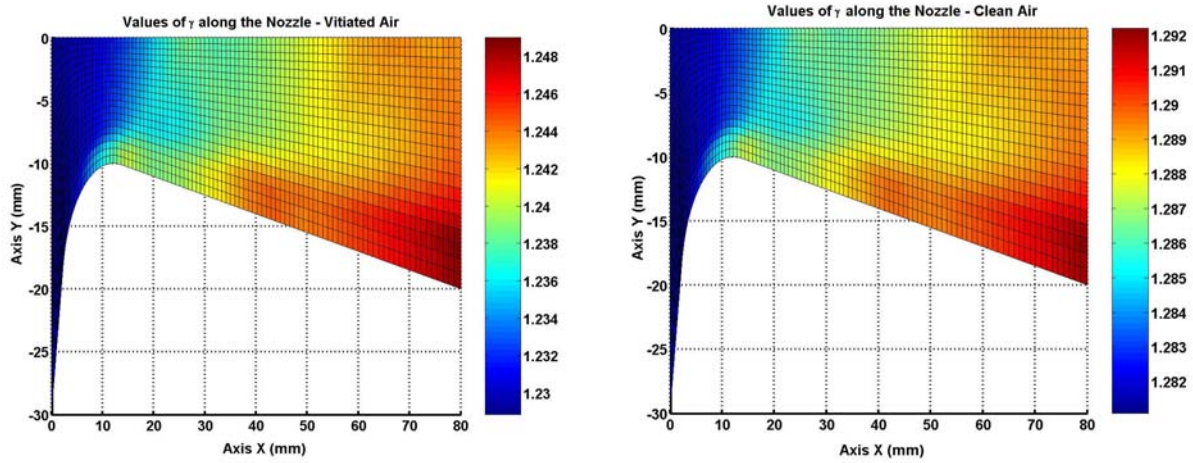


Figure 11: Distribution of γ values for the vitiated and the clean air along the nozzle.

The work presented here is a short version of the complete study of the flow conditions inside a supersonic combustion ground test facility (Leite, 2006). The main goal was to create a tool to predict the inlet flow conditions, at the facility entrance, to obtain the desired properties of the test flow, at its exit, for each different case to be simulated. This way it is possible to generate and control the desired flow test conditions by manipulating the mass flow rates of fuel, air and O_2 at the facility entrance only.

4. REFERENCES

Anderson Jr., J. D., 1990, "Modern Compressible Flow", McGraw-Hill Book Co, New York.
Anderson Jr., J. D., 1995, "Computational Fluid Dynamics", McGraw-Hill Book Co, New York.
Anderson Jr., J. D., 2000, "Hypersonic and High Temperature Gas Dynamics", AIAA, Reston, VA.
Andrews, E. A. Jr. et al., 1985, "Langley Mach 4 Scramjet Test Facility", NASA TM-86277.
Baranovskii, S. I. et al., 1988, "A Simple One-Dimensional Model of the Air Contamination Effect on Supersonic Combustion", Explosion and Shock Waves, 24 (6), pp. 677-685.
Boyce, R. R. et al., 1998, "Supersonic Combustion - A Shock Tunnel and Vitiation-Heated Blowdown Tunnel Comparition", 36th Aerospace Sciences Meeting and Exhibit, Reno, NV.
Cathonnet, M., 2003, "Advances and Challenges in the Chemical Kinetics of Combustion", European Combustion Meeting, Òrleans, Anais…, França.
Curran, E. T., 2001, "Scramjet Engines: The First Forty Years", Journal of Propulsion and Power, vol. 17, nº 6, pp. 1138-1148.
Curran, E. T. et al, 1996, "Fluid Phenomena in Scramjet Combustion Systems", Annu. Rev. Fluid. Mech.
Degaut, P. et al., 1994, "Kerosene Combustion at Pressures up to 40 atm: Experimental Study and Detetailed Chemical Kinetic Modeling", 25th Symposium (International) on Combustion/Combustion Institute, Anais…**,** Pittsburgh, PA.
Degaut, P., 2002, "On the Kinectics of Hydrocarbons Oxidation from Natural Gas to Kerosene and Diesel Fuel", Physical Chemistry Chemical Physics, v. 4, pp. 2079-2094.
Gruber, M. et al., 2001, "Newly Developed Direct-Connect high-Enthalpy Supersonic Combustion Research Facility", Journal of Propulsion and Power, vol. 17, nº 6, pp. 1296-1304.
Guimarães, A. L. S., 1996, "Modelagem de um Aquecedor para Banco de Testes de Estato-Reatores a Combustão Supersônica", MSc. Dissertation, National Institute for Space Research (INPE), São José dos Campos, Brazil.
Guy, R. W. et al., 1996, "The NASA Langley Scramjet Complex", AIAA, ASME SAE and ASEE, 32nd Joint Propulsion Conference and Exhibit, Lake Buena Vista, FL.
Jameson, A.; Schmidt, W.; Turkel, E., 1981, "Numerical solution of the euler equations by finite volume methods using runge-kutta time-stepping schemes". Paper AIAA-81-1259.
Kee, R. J. et al., 2000, "Aurora: a Program for Modeling Well Stirred Plasma and Thermal Reactors with Gas and Surface Reactions in Steady or Transient Conditions", Reaction Design. Inc., San Diego, CA.
Kee, R. J. te al., 2000, "Plug: a Program for the Analysis of Plug-Flow Reactors with Gas-Phase and Surface Chemistry: Reaction Design. Inc., San Diego, CA.
Leite, V. S. F. O., 2006, "Caracterização do Escoamento de uma Bancada ds Testes de Combustores Supersônicos Alimentada por Ar Viciado", Ph.D. Theses, Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil.
Lewis, M. J., 2001, "Significance of Fuel Selection for Hypersonic Vehicle Range". Journal of Propulsion and Power, v. 17, n. 6, pp. 1214-1221.
Li, S. C.; Varatharajan, B.; Williams, F. A., 2001, "Chemistry of JP-10". AIAA Journal, v. 39, n. 12, pp. 2351-2356.
Marshall, G, 2002, "Scram!", Popular Science Aviation/Space. October 2002. 1 ilustração, color. Available at <http://www.popsci.com/popsci/aviationspace/91295b4a1db84010vgnvcm1000004eecbccdrcrd/4.html>.
Masuya, G. et al., 1995, "Ignition and Combustion Performance of Scramjet Combustors with Fuel Injection Struts", Journal of Propulsion and Power, vol. 11, nº 2, pp. 301-307.
Mcbride, B. J. et al., 1963, "Thermodynamic Properties to 6000 K for 210 Substances Involving the First 18 Elements". NASA SP-3001, NASA Langley Research Center, Hampton, VA.
Montgomery, C. J. et al., 2002, "Reduced Chemical Kinetic Mechanisms for JP-8 Combustion". In: 40th Aerospace Sciences Meeting And Exhibit, 2002, Reno, NV. Anais… Reno, NV. (Paper AIAA 2002-0336).
Petrobrás, 2000, "Especificação de Querosene de Aviação (QAV-1)", Portaria ANP Nº 137, Brasília, DF.
Petrobrás, 2005, "Especificação do querosene de aviação (QAV-1)", October 2005, Available at <http://www.br.com.br/portalbr/calandra.nsf#http://www.br.com.br/portalbr/calandra.nsf/0/4B9907EC3CD0940303256C5C00713B56?OpenDocument&Saviacao>.
Pulliam, T. H., 1986, "Artificial Dissipation Models for Euler Equations", AIAA Journal, v. 24, n.12, pp. 1931-1940.
Purvis, 2001. "Modern US Military Turbine Missile Fuel Specifiction", June 2004, Available at <http://purvisbros.com/afi/modernmilturbinemissle.htm>.
Rogers, R. C.; Capriotti, D. P.; Guy R. W., 1998, "Experimental Supersonic Combustion Research at Nasa Langley", NASA Langley Research Center, AIAA paper 98-2506.

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