Ramjet NOx Emission
Use of a 3D CFD Method for the Combustor Design of a Super/Hyper-Sonic Transport Propulsion System

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ABSTRACT

As part of SNECMA participation in developing the ramjet of Large-Scale Japanese Project for "SUPER/HYPER-SONIC TRANSPORT PROPULSION SYSTEM", an injection system of lean premix type has been studied.

This concept based on a low fuel/air ratio combustion allows a high reduction of NOx emission. Fuel and air mixing must be rapid and homogenous in order to obtain the full potential of this principle.

For that purpose, a numerical study has been carried out to find the optimal mechanism on carburation homogeneity. Results of a parametric study are presented and show influences of various injection and flame holder systems on air/fuel flow distributions.

Numerical simulations have been performed with the 3D CFD ECRIN code. It is commonly used at SNECMA for combustion analysis. The main features of this code are presented and more particularly the combustion and NOx emission modeling. A comparison of calculated NOx emission indexes with experimental results obtained in a tubular combustor conducts to a good agreement between experiments and computations.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc</td>
<td>Blockage Ratio</td>
</tr>
<tr>
<td>EINOx</td>
<td>NOx Emission Index (g of equivalent NO2 / kg of Fuel)</td>
</tr>
<tr>
<td>FF</td>
<td>Total Fuel</td>
</tr>
<tr>
<td>FF</td>
<td>Variance of FF</td>
</tr>
<tr>
<td>i,j,k</td>
<td>Node Coordinates in Computational Domain</td>
</tr>
<tr>
<td>lt</td>
<td>Turbulent Length Scale (m)</td>
</tr>
<tr>
<td>m_e</td>
<td>Mass Flow in Each Cell n</td>
</tr>
<tr>
<td>N</td>
<td>Number of Injection Points</td>
</tr>
<tr>
<td>NOx</td>
<td>Oxides of Nitrogen</td>
</tr>
<tr>
<td>P(FF)</td>
<td>Presumed Probability Density Function of Total Fuel</td>
</tr>
<tr>
<td>R, Z, Θ</td>
<td>Coordinate System in Physical Domain</td>
</tr>
<tr>
<td>ρ</td>
<td>Density of the Flow</td>
</tr>
<tr>
<td>V</td>
<td>Percentage of Ramjet Volume with 0.5 &lt; Φ &lt; 1.2</td>
</tr>
<tr>
<td>YNO</td>
<td>Arrenhius Rate of Formation of NO</td>
</tr>
<tr>
<td>Y NO</td>
<td>Mass fraction of NO</td>
</tr>
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</table>

Greek symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>c</td>
<td>YNO / YNO equilibrium</td>
</tr>
<tr>
<td>ε</td>
<td>Dissipation Rate</td>
</tr>
<tr>
<td>Φ</td>
<td>Equivalence Ratio</td>
</tr>
<tr>
<td>Φ_e</td>
<td>Equivalence Ratio in Each Cell n</td>
</tr>
<tr>
<td>Φ_a</td>
<td>Average Equivalence Ratio</td>
</tr>
<tr>
<td>σ</td>
<td>Mass-Weighted Standard Deviation of Equivalence Ratio</td>
</tr>
</tbody>
</table>

INTRODUCTION

In order to reduce significantly flight time, the Supersonic Transport has been reinvestigated by the aeronautical community and active researches and developments for Super/Hyper-sonic Transport (SST/HST). With this aim, a Large-Scale Project has been initiated by Japan in 1989 to develop basic technologies. Foreign big engine manufacturing companies are also interested in this project.

In this challenging program SNECMA contributes to the design of a ramjet engine at stratospheric cruise conditions with low pollutant emission levels. So, the SST/HST will become a reality if, among other things, nitrogen oxide emissions remain comparable with NOx emissions of future aircraft.

For that purpose, an injection system of Lean Premix type has been numerically studied.
This concept based on a low fuel/air ratio combustion allows to reduce NOx emission level by avoiding local heterogeneities (Ferri, 1972, Bayle-Laboure, 1986). Indeed, the rate of change of NO depends largely on local temperatures, residence time and shows a significant peak for stoichiometric mixtures. Furthermore, fuel and air mixing must be rapid and homogeneous in order to obtain the full potential of this principle (Roffe et al., 1976, Fiorentino et al., 1980).

In this study only ramjet geometry and cruise conditions were given. Flame stabilizing and fuel injection having a major influence on NOx emissions for a lean premix system, a parametric study was performed in order to rank several concepts in regard to pollutant emissions.

The present formulation of the problem shows that the ramcombustor design depends on physical and geometric parameters and parameters linked to fuel injection system. Results concerning some of these parameters are presented in the first section. A discussion about air/fuel flow distributions and the importance of stoichiometric zones, which are directly influential in NOx emission, is proposed.

The second section of this paper describes the validation of the SNECMA ECRIN code NOx prediction model. This code commonly used at SNECMA (Karadimas, 1989) to calculate combustor flows has been validated on a wide range of configurations. Some additional work is described here that has been done on SNECMA tubular combustors. Its aim is to verify the predictability of the NOx model and the potential of such a model to make quantitative evaluation of pollutant level in terms of NOx emission indexes (EIN0x).

THE 3 D CFD ECRIN CODE

The 3D ECRIN code is commonly used at SNECMA for combustion analysis. The main characteristics of this turbulent reacting flow simulation code are :

- Cartesian structurated mesh
- Finite volume formulation
- Staggered grid
- SIMPLE algorithm
- Semi-implicit formulation
- Time dependent
- FCT technique to control numerical diffusion.

The models included in ECRIN are :

- Standard K-c turbulence model
- 4 steps chemical kinetic scheme with 8 species
- Eddy Break Up - Arrhenius model for turbulence / chemical kinetics interaction
- Wall log laws
- Six flux radiation model
- Diphasic lagrangian formulation.

This code has been validated on many configurations including classical and academic test cases. SNECMA has been using it on industrial configurations (combustors, afterburners and underexpanded jets) for more than 5 years.

RAMJET DESIGN - NUMERICAL SIMULATIONS

Position Of Problem

3D numerical predictions are performed on a cylindrical geometry. In a combined cycle engine concept, only the ramjet has to be simulated at cruise conditions (M=5). Combustion is described by a turbulent modeling of propane oxidation. Due to geometric symmetry, computational (R-Q) domain is limited to a circular section with an angle of 45 degrees.

The flame stabilization system located in the ramjet has been designed in order to reduce NOx emission level by avoiding local heterogeneities. Only one configuration of flameholder (baseline flameholder) is presented in this paper.

Grid

The mesh used in the current computations involves 62, 34, 17 nodes in Z, R, θ directions respectively. The grid shown in Figure 1 is obtained in the θ midplane (Fig.1a) and in baseline flame holder plane (Fig.1b).
Numerical Procedure

The steady state of reacting flow fields is obtained by solving transport equations of \( u, v, w \) - momentum, pressure, turbulent kinetic energy \( K \), dissipation rate \( c \), total enthalpy and mass fractions. Variable fluid properties (i.e. temperature and pressure dependency of density, temperature dependency of specific heat, laminar viscosity...) are taken into account in computations.

A standard K-\( e \) model with wall functions is used with turbulent Prandtl and Schmidt numbers of 0.7.

Walls are supposed adiabatic.

The oxidation of propane is described by a Four-Step scheme and seven active chemical species are numerically deduced.

Convergence of the numerical solution is checked by monitoring selected variables at each time step. Computations are performed on an AMDHAL 5990-1400 supercomputer.

Boundary Conditions

The pure air stream inlet conditions are:

- Axial Velocity = 50 m/s
- Temperature = 1330 K
- Pressure = 6 b

A uniform velocity profile is assumed. Turbulent kinetic energy and turbulent length scale are variable parameters.

The composition at the fuel injection is supposed to be propane at 400 K. The global equivalence ratio is about 0.3. Fuel injection points are numerically represented by source points assuming a given mass flow rate.

The outlet boundary condition is a zero gradient boundary condition.

No-slip adiabatic wall conditions are assumed. The centerline is supposed to be a symmetry axis with a zero gradient boundary condition except for the \( v \)-component of the velocity which is assumed to be 0.

Grid Independence

In order to test grid independence, computations were performed with two different sizes of grids : 35836 and 93279 cells. The \( U \)-isocomponents of the velocity (Figure 2) were chosen as the test of the two meshes. Computational results with the coarse and fine grids are very similar. It appears that the coarsest mesh capture very well the overall physics of the current problem and can be used to find the optimal mechanism on carburation homogeneity.

![Fig. 2. Comparison of U-isocomponents of the velocity for coarse and fine grids.](https://proceedings.asmedigitalcollection.asme.org)

Key Parameters

The formulation of the problem shows that the low emission ramcombustor design depends on several parameters. Some of these key parameters are presented and ranked as follows:

- **Physical parameters**
  - Upstream turbulent kinetic energy
  - Upstream turbulent length scale

- **Geometric parameters**
  - Flame stabilization concept
  - Flameholder shape and location
  - Blockage ratio

- **Injection parameters**
  - Number of injection holes
  - Angle of fuel injection
  - Location of injection system

Numerical Result Analysis Procedure

The production of NOx during combustion is extremely sensitive to:

- Temperature level and equivalence ratio value
- Air/fuel mixing

Therefore, in order to examine effects of each key parameter on NOx emission, both parameters mentioned above have to be evaluated (Fletcher et al., 1971).

In present computations assuming that chemical equilibrium is obtained (except for NO) temperature and equivalence ratio distributions are homothetic. Consequently only a discussion about equivalence ratio has to be done.

Two parameters are used in order to estimate the performance of systems in regard to NOx emission:

- The first is the percentage of ramjet volume (V) for which \( 0.5 < \phi < 1.2 \). As stoichiometric equivalence ratio, and therefore high temperature zones, have to be avoided, the smallest value of this parameter is required in order to reduce NOx emission.

- The second is the mass-weighted standard deviation of equivalence ratio \( (\phi_{\sigma}) \) which is calculated for each computation. \( \phi_{\sigma} \) is given by:

\[
\phi_{\sigma} = \sqrt{\frac{\sum m_n (\phi_n - \phi_{\bar{\phi}})^2}{\sum m_n \phi_n}}
\]

(1)

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With $\bar{\phi}$, the equivalence ratio average value. As a quasi-homogeneity of the mixing is researched, the smaller is $\bar{\phi}$ the better is the quality of the mixing.

**Numerical Results**

In this section only the effects of turbulent length scale ($lt$), blockage ratio ($BC$) and number and location of the injection holes ($N$) on NOx emission in a ramjet are considered.

Figures 3 to 6 are shown to provide a qualitative approach of the air/fuel homogeneity and the stoichiometric equivalence ratio zone distributions. Indeed these graphs give the ratio of ramjet volume having the same equivalence ratio over the total ramjet volume. The baseline configuration ($lt = 0.1$, $BC = 0.32$, $N = 12$), around which influence of the three parameters $lt$, $BC$ and $N$ are studied, is presented in Figure 3.

**Effect of Turbulent Length Scale ($lt$).** Although the parameter $lt$ is difficult to control and to determine, it is interesting to define its influence (Al Dabbagh et al. 1983). $lt$ represents the upstream turbulent scale. It can be calculated according to:

\[
lt = \frac{N \cdot Deq}{2}
\]

with $N \in [0.1 - 0.4]$ and $Deq$ the inlet characteristic dimension. Three values of $lt$ are chosen: 0.05m, 0.1m and 0.15m. The results of $lt$ effect on NOx emissions through $\bar{\phi}$ and $V$ are assembled in table 1.

**Table 1: Effect of turbulent length scale on flow distribution parameters**

<table>
<thead>
<tr>
<th>$lt$</th>
<th>$\bar{\phi}$</th>
<th>$V$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.6173</td>
<td>11.03</td>
</tr>
<tr>
<td>0.10</td>
<td>0.5217</td>
<td>6.73</td>
</tr>
<tr>
<td>0.15</td>
<td>0.4887</td>
<td>6.20</td>
</tr>
</tbody>
</table>

As turbulent length scale is increased from 0.05 to 0.15, the mixing parameter $\bar{\phi}$ and the volume fraction $V$ are reduced respectively of 26% and 78%. As can be seen in Figure 4, air/fuel distribution is more homogeneous and well centered around the global equivalence ratio for $lt = 0.15$ (Fig.4b) than for $lt = 0.05$ (Fig.4a). A strong effect of vortex size can be noticed which is very influential in NOx emissions (Al Dabbagh et al., 1983).
Effect of Blockage Ratio (BC). Flame stabilizing pressure loss is a major factor influencing fuel and air mixing and therefore NOx emissions. Thus, blockage ratio is a relevant parameter to investigate. For this study, flameholder shape is kept and only the blockage ratio is variable. A large range of BC values is presented in Table 2.

<table>
<thead>
<tr>
<th>BC</th>
<th>α#</th>
<th>V (%)</th>
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<tbody>
<tr>
<td>0.2</td>
<td>0.5482</td>
<td>9.53</td>
</tr>
<tr>
<td>0.25</td>
<td>0.5442</td>
<td>7.96</td>
</tr>
<tr>
<td>0.32</td>
<td>0.5217</td>
<td>6.73</td>
</tr>
</tbody>
</table>

Table 2: Effect of blockage ratio on flow distribution parameters

As BC is enhanced, the mixing homogeneity is improved. Furthermore, the percentage of ramjet volume with equivalence ratios close to stoichiometry is smaller. Therefore, expected NOx emission will be the lowest for BC = 0.32. Figure 3 (BC = 0.32) shows a more Gaussian shape than the ones obtained for BC = 0.2 (Fig. 5a) and for BC = 0.25 (Fig. 5b). That indicates a more homogeneous air/fuel mixing. Indeed, for a high blockage ratio value recirculations induced by flameholder are more important and contribute to a better air/fuel mixing.

Effect of number and location of injection holes (N). To study this parameter, fuel is injected in streamwise and parallel to the air flow. Fuel injection points are numerically represented by source points assuming a given mass flow rate. Three values of the parameter N are tested (6, 12, 24) with various fuel injection locations in the 0 planes (represented by the k coordinates in the computational domain).

<table>
<thead>
<tr>
<th>N</th>
<th>α#</th>
<th>V (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 x 6 holes in k = 9</td>
<td>0.7497</td>
<td>31.2</td>
</tr>
<tr>
<td>2 x 6 holes in k = 5,13</td>
<td>0.5217</td>
<td>6.73</td>
</tr>
<tr>
<td>4 x 6 holes in k = 4,14</td>
<td>0.6020</td>
<td>9.74</td>
</tr>
<tr>
<td>4 x 6 holes in k = 4,7,11,14</td>
<td>0.5153</td>
<td>12.8</td>
</tr>
<tr>
<td>4 x 6 holes in k = 4,5,13,14</td>
<td>0.5210</td>
<td>7.03</td>
</tr>
</tbody>
</table>

Table 3: Effect of number and location of injection holes on flow distribution parameters

Table 3 shows that the influence of the number and the location of injection points is very pronounced. A fuel injection in the 0 midplane is drastically unfavorable. The percentage of ramjet volume with quasi-stoichiometric equivalence ratios is very important (31%). In terms of NOx emissions this concept seems very detrimental. An increase of the number of injection points is more favorable provided that these holes are very close. That is shown in Figures 6a and 6b on which are respectively reported distributions of ramjet volume as a function of φ for N = 6 (k = 9) and N = 24 (k = 4-7-11-14). A large fraction of ramjet volume with φ > 0.5 can be observed (Fig. 6a). Therefore this injection concept would produce more NOx. For N = 24 (Fig. 6b) a more pronounced peak appears around φ but a greater volume can be noticed in stoichiometric zones. Thus, a compromise between the number and the location of fuel injection points is to be found in order to obtain the more attractive configuration as far as NOx reduction is concerned.
The Thermal Nitrogen Oxide Model

Due to the high operating conditions for temperature and pressure in aircraft combustor (P > 10 bar, T > 2000 K) and during combustion of lean and near stoichiometric fuel-air ratio, nitrogen oxide forms mainly via the so called thermal way which is generally described by the extended Zeldovitch mechanism. This model is a representation of the kinetic oxidation of atmospheric nitrogen catalysed by temperature and particularly by temperature greater than 1900 K. Therefore, the concentration of NO obtained by this model is a strong function of oxygen and nitrogen concentrations, fuel-air ratio and residence time.

The Zeldovitch Mechanism (Miller et al., 1989)

\[
\begin{align*}
N_2 + O & \rightleftharpoons NO + N \quad (3) \\
N + O_2 & \rightleftharpoons NO + O \quad (4) \\
N + OH & \rightleftharpoons NO + H \quad (5)
\end{align*}
\]

The reaction (3) is endothermic left to right and relatively slow, whereas the reactions (4) and (5) are exothermic and fast. Without any simplification the rate of change of NO can be derived as follows:

\[
d[NO]/dt = k_1[N_2][O] - k_1[NO][N] + \\
k_2[N][O_2] - k_2[NO][O] + \\
k_3[N][OH] - k_3[NO][H]
\]

where \([\cdot]\) denotes concentrations in mole/m³. \(k_{1+}^{+/-}\) are the forward and reverse constants of the ith reaction.

To compute the reaction rate of NO, some assumptions have to be done in order to get the \([O], [OH], [H]\) and \([N]\) concentrations which are not calculated by the fuel chemical kinetic scheme.

First assumption. The steady state assumption is made for N (\(d[N]/dt=0\)) because the atomic nitrogen is in very small amount compared with the other concentrations of interest.

Second assumption. At the typical running conditions (temperature and pressure) of a gas combustor, the chemical reactions are very fast compared with residence time and turbulence characteristic time. An appropriate assumption is therefore that \([O], [O_2], [OH]\) and \([H]\) concentrations and temperature are the equilibrium values.

With these assumptions, the rate of change of NO is written as follows:

\[
W_{NO} = dY_{NO} / dt = K_1 \frac{1 - \alpha^2}{1 - K \alpha} \quad (7)
\]

\(\alpha = Y_{NO} / Y_{NO \text{ equilibrium}}\)

where \(Y_{NO}\) is the mass fraction of NO

To design low emission combustor a 3D computational method for NOx has been performed with the 3D computational fluid dynamics SNECMA ECRIN code.

An application on a tubular combustor is done in the following.

MODELING OF THE NITROGEN OXIDE EMISSIONS FROM AN EXPERIMENTAL TUBULAR COMBUSTOR

It is now well known that the combustion of fuel conducts to nitrogen oxide production. Its formation involves in varying extents the three routes, namely thermal, prompt and fuel-nitrogen. These processes are interlinked and depend mainly on fuel composition, fuel-air ratio, temperature and residence time. In order to reduce the NOx emissions of future aeronautic combustors, new technologies have to be developed.
program. The evolution of the rate of change of NO versus time has been calculated and is presented in Figure 7.

![Graph showing rate of change of NO versus time](image)

**Fig. 7.** Arrhenius rate of change of NO with equilibrium assumption.

\[ W_{NO} \text{ is therefore only a function of the mass fraction of NO and of the "total fuel"} \]

\[ \text{Mass of all carbon species count in equivalent fuel} \]

\[ \tilde{FF} = \frac{\text{FFmax}}{\text{total mass}} \]

The turbulent fluctuations are taken into account by a presumed probability density function of the variable FF.

Four forms are possible for the presumed pdf, \( P(FF) \), depending on the mean value FF and its variance \( FF^2 \), which are solved by two homogeneous transport equations (Bray et al., 1985, Champion et al., 1978, Moreau, 1980,).

The mean reaction rate of NO can therefore be written as follows:

\[ W_{NO} = \int_{FF_{min}}^{FF_{max}} P(FF) W_{NO} (Y_{NO,FF}) dFF \]

**Comparison Between Calculations And Measurements**

Numerical procedure. This NOx prediction model in turbulent flow field is tested on an experimental tubular combustor representative of an industrial combustor, on which NOx measurements for three running conditions (pressure and temperature) are available (Table 4).

Once the converged reactive flow field is obtained, containing the mean value of FF, the transport equations for \( FF^2 \) and for NO are solved. Some numerical tests show that the convergence of FF and therefore the local pdf form determination is rapidly obtained compared to NO value. This is mainly due to the fact that FF and \( FF^2 \) are homogeneous whereas the transport equation for NO presents a very stiff RHS term representing the production term. Therefore the calculations are monitored by checking the convergence rate of NO (Figure 8).

![Numerical results: tubular combustor P = 3 bar, T = 532 K.](image)

(a) Velocity field  
(b) Temperature  
(c) NO Mass fraction

**Fig. 8.** Numerical results: tubular combustor P = 3 bar, T = 532 K. (a) Velocity field  
(b) Temperature  
(c) NO Mass fraction
Numerical results. The comparison between calculations and measurements are given in the following table (Cadiou, 1991):

<table>
<thead>
<tr>
<th>Inlet conditions</th>
<th>EINOx experimental</th>
<th>EINOx calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>P = 3 bar, T = 532 K</td>
<td>0.840</td>
<td>0.997</td>
</tr>
<tr>
<td>P = 7 bar, T = 657 K</td>
<td>1.012</td>
<td></td>
</tr>
<tr>
<td>P = 20 bar, T = 777 K</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4: Inlet conditions, EINOx experimental and calculated ratio.

This model conducts to a very good prediction of the NOx emission level in the tubular combustor, particularly at high pressure (Table 4). The assumption of chemical equilibrium is more accurate at high pressure than at low pressure. Therefore the production of NO is over-estimated at low pressure. That could explain the larger discrepancy with experimental/calculated EINOx ratio obtained at P=3 bar and T=532 K.

CONCLUSION

From the results obtained by the SNECMA ECRIN code, the following conclusions may be made for the ram combustor design for given geometry and cycle conditions:

- The turbulent length scale has a great impact on the mixing, hence the evaluation of this parameter at the entrance of the combustor is important.
- As blockage ratio is enhanced the expectable NO emission level is lower.
- An increase of the number of injection points is favorable provided that these holes are very close.

The prediction of the NOx emission levels on the three SNECMA experimental cases extracted from our database validation shows clearly that a quantitative evaluation of EINOx can be obtained on industrial cases through the use of a 3D simulation. As soon as a combustor geometry is sufficiently well defined such computations can be made. This tool will be very useful to characterize the performance of the future SST/HST ramjet as far as NOx emissions are concerned.

ACKNOWLEDGEMENTS

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