ABSTRACT
This paper deals with the very last activities carried out by EnginSoft in the frame of the EU funded research programme NEWAC. The work regards the pre-production numerical tests performed on the single annular combustor with the purpose of verify its performance in reactive frame. The core of this study is the innovative lean-burn injection system technology, developed by University of Karlsruhe and AVIO for medium OPR. Such device has been widely investigated in previous activities in order to optimise the combustor layout and the numerical procedure for this work [1].

INTRODUCTION
NEWAC is an initiative from the European aero engines manufacturers, the main European aircraft manufacturer (Airbus), SMEs and industry providing innovative technologies and leading research institutions in the field of aeronautics to provide a step change for low emission engines. In order to pursue the goal, NEWAC addresses to the development of innovative engine core configurations.

In this frame AVIO is responsible of the medium OPR combustor design and manufacturing, coordinating a team of European Universities (University of Karlsruhe, University of Florence) Centre of Research (ONERA, CEPr) and engineering companies (EnginSoft).

State of the art of Aero Engines
Global air traffic is estimate to grow at an average annual rate of about 5% in the next 20 years. The gases and particles emitted by the engines contribute to local air quality degradation in the airport neighbourhood and alter the concentration of greenhouse gases on a global level, leading to climate change. Large investments have already been made in Europe and the US through R&D programmes and collaborations to reduce the negative environmental effects of aircraft use. To reduce NOx and CO2 emissions to achieve the ACARE objectives it is indispensable to develop new engine configurations and to perform complementary research and development of core engine technologies.

NEWAC Objectives
ACARE identified the research needs for the aeronautics industry for 2020, as described in the ACARE Strategic Research Agenda. The following targets regarding the aero engines are set, which will be looked for by NEWAC:

- 20% reduction in CO2 emissions per passenger-kilometre whilst keeping specific weight of the engine constant (see Figure 1);
- significant reduction of the NOx emissions during the landing and take-off cycle (-80%) and in cruise (-60%) respect to CAEP/2 limit (see Figure 2).
The main result of NEWAC will be fully validated, novel technologies enabling a 6% reduction in \( CO_2 \) emission and a 16% reduction in \( NO_X \) respect to EEFAE results, according to ICAO Landing and Take-Off (LTO) cycle. In particular the specific objectives of the Sub-Project SP6 are to develop and validate lean fuel injection technology up to TRL 5-6, demonstrating from 60% to 70% reduction of \( NO_X \) emissions in the LTO cycle versus CAEP/2 limit. These results will be integrated with past and existing EC projects in the field, notably EEFAE, VITAL and national programmes, thus \( CO_2 \) can be reduced up to 20% and \( NO_X \) close to 80%, hence enabling European manufacturer to attain the ACARE 2020 global targets.

The project will address the particular challenge to deliver these benefits simultaneously: many technological developments based on conventional thermodynamic cycles are driven to high temperature and pressure levels to reduce \( CO_2 \) whilst compromising \( NO_X \) emissions. To avoid this conflict a number of innovative core engine concepts will be investigated and key components will be tested and evaluated. In particular, all these engine concepts are based on single annular combustor architecture. The most important advantage offered by a single annular combustor layout is its high potential to keep low the costs and weight associated with the introduction of low emission combustion technology. The innovative core concepts needed to support are:

- low to high OPR
- medium to high thrust
- short to long range

Different operating conditions have need of different engine sizes; therefore the improvement of different lean burn fuel injection concepts is also required.

**Global objectives**

NEWAC programme can be seen as part of the European long-term technology goals about low emission combustion. Two main goals are set in this frame:

- strengthening the competitiveness of European aero-engine OEMs by means of reduce short (-20%) and long (-50%) term development costs, incorporate new technologies faster into future products and reduce project timescales to less than 2 years;
- improving the environmental impact with regards to emissions through EC FP6 Aeronautics Work Programme (-80% \( NO_X \) emissions respect to CAEP/2 ICAO-LTO cycle, achieving a \( NO_X \) emission index of 5 g/kg\(_{FUEL}\) in cruise) and ACARE “A Vision for 2020” (-50% \( CO_2 \) emissions, of which 15-20% by engine contribution, and strong \( NO_X \) emissions, -80% total and -60% in cruise).

**Innovative Combustor**

The combustion systems is the only contributor for \( NO_X \) emissions.

All promising approaches for significant \( NO_X \) emission reduction are on the basis of lean premixing combustion technology. Demonstrator engines equipped with this technology attested the \( NO_X \) reduction potential. Additional improvement (especially fuel injection technology) is required to enable the ACARE 2020 targets. The real challenge is the contemporaneous demand of \( CO_2 \) reduction targets: more efficient aero-engine cycles for reducing specific fuel consumption usually result in higher loaded core engines burdening the combustion system with higher entry pressures and temperatures and the risk for even higher \( NO_X \) emissions. In principle, lean combustion compromises combustor operability, including ignition, altitude relight, pull-away, weak extinction performance and thermo-acoustic instability behaviour. To overcome these shortfalls lean combustion is integrated into fuel staged combustion concepts increasing the complexity, costs and weight significantly compared to conventional combustion systems.

**FIGURE 1: FUEL CONSUMPTION / \( CO_2 \) REDUCTION FOR DIFFERENT CORE CONCEPTS: NEWAC VS. STATE OF THE ART**

**FIGURE 2: NOX REDUCTION FOR DIFFERENT CORE CONCEPTS: NEWAC VS. STATE OF THE ART**
Lean combustion technology operates with an excess of air to significantly reduce flame temperatures and consequently decrease NO\textsubscript{X} formation. For this reason, up to 70\% of the total combustor airflow has to be premixed with the fuel before entering the reaction zone within the combustor module. Therefore, cooling flow has to be reduced accordingly to provide sufficient air for mixing. The optimisation of homogeneous fuel-air mixtures is the key to achieve lower flame peak temperatures and lower thermal NO\textsubscript{X} formation. However, this homogenisation has a strongly adverse effect on combustion lean stability, drastically narrowing the operating and stability range. To overcome these stability drawbacks while maintaining good NO\textsubscript{X} performance, fuel staging is required: this can be made by internally staged injectors in a single annular combustor architecture creating a pilot line and a main line with fuel film formation combustion zone downstream of a common fuel injector. The advantage of a staged combustor is that each zone can be optimised for a particular requirement (regarding different parts of the flight envelope).

Different enabling technologies are required for reaching low NO\textsubscript{X} combustion system targets, particularly addressed to the cooling air reduction and the fuel staging:

- cooling technology with significant cooling flow reduction;
- stability control system to maintain combustor operability;
- control of thermo-acoustic and combustion instabilities;
- staged fuel and control system for the pilot and main injection circuits to control the flame temperature and the NO\textsubscript{X} emissions.

**ENGINSOFT: 3 YEARS ACTIVITY IN NEWAC**

EnginSoft is active with its CFD team in combustion activities for aero-engines for more than a decade. Particularly the team has been active in EU funded research projects as well as several engineering consultancies investigating reacting flows with different physical models, optimising injector geometries, verifying recirculation and flame stability and finally focusing on low emissions. In the past, EnginSoft has been involved in activities within ANTLE and CLEAN programme for heat transfer and combustion optimisation applications. Such activities were also one of the first to employ the novel developed optimisation platform modeFRONTIER for industrial applications. Thanks to its wide expertise on CAE (process simulation, CFD, optimisation of design), EnginSoft is one of the 40 partners of NEWAC. The main role of EnginSoft in NEWAC within SP6 is to bring a contribution to the CFD design of Ultra Low NO\textsubscript{X} AVIO Single Annular Combustor, by means of:

- Flow field verification of an innovative lean injection system, designed by University of Karlsruhe and AVIO, applied for medium overall pressure ratios (20 < OPR < 35). The device consists of a co-rotating double swirler centripetal injector (see Figure 3). This technology is addressed to achieve partial evaporation and rapid mixing within the combustor, optimising the location of the flame and the stability of the lean system. The purpose of CFD analysis and experimental tests on injection system is to individuate the swirler working flow function, hence the mass flow required in order to reduce emissions under the available pressurisation (depending on engine layout) and to verify that injection system provides good mixing and recirculation for flame stability. In particular, the aim of this activity is to point out any meaningful difference on the injection system performance, depending on boundary conditions (pressure drop vs. mass flow), plenums sensitivity (the downstream chamber shape strongly affect air distribution) and transient vs. steady state flow field. Turbulence model sensitivity has been performed too. Among the 2-equations turbulence models, the Shear Stress Transport (SST) gives the best matching with experimental measurements.

- Optimization of the external flow field of the Ultra Low NO\textsubscript{X} combustor chamber, focusing on the optimisation of some specific component like cowl, bleeds and fuel tube keel. In particular, a preliminary CFD optimisation has been performed on a simplified 2D geometry of the combustor; this study provides a general suggestion of the behaviour of the fluid upstream the combustor chamber due to the cowl shape. Also here, turbulence model sensitivity has been performed. The best layouts show no separation at cowl edges and no counterproductive recirculation in the diffuser.

**FIGURE 3: LEAN INJECTION SYSTEM - STREAMLINES**

Then, the results derived from the preliminary 2D study have been applied in a 3D investigation on a periodic sector of the complete annular combustor (see Figure 4).
The main objective in this stage is to reach the best layout for dilution holes in order to optimise the combustion process. Acting on holes diameter and position it is possible to change air distribution and dilution flow diffusion: these aspects contribute to create a recirculating region that guarantees flame stability and for cooling.

Several layouts have been investigated by EnginSoft in order to give a prediction of the behaviour of the device. The attention has been focused on different aspects, as:

- air split between swirler vanes, dilution holes and bleed holes (for turbine air cooling supply);
- pressure distribution in the inner/outer annulus and in the combustion chamber;
- fuel tube wake in the outer annulus;
- recirculation region in the combustor chamber.

A comparison between k-ε and SST turbulence models has also been considered. Since in this application the recirculating region has a fundamental influence on the behaviour of the device, the SST turbulence model is preferred because the weakness of the k-ε model in the late prediction of the onset of separation and the under-prediction of the amount of the separated region.

Two operating conditions have been considered in order to cover a wide pressure range and, consequently, to have a robust definition of all the adopted settings. The considered operating points are reported in Table 1.

![FIGURE 4: COMPLETE COMBUSTOR](image)

- Robust design of the combustion flow field in order to verify the exhaust temperature. The numerical activity performed by EnginSoft has been split into two stages:

1. CFD software evaluation on a simple reactive tubular test rig model ⇒ the aim of this stage is to assume and tune the correct numerical models and parameters to fit experimental data acquired by ONERA Laboratory (temperature profiles in particular). The test rig device has been developed by ONERA Laboratory to evaluate the lean injection system performance in combustion frame. The system, shown in Figure 5, consists of upstream and downstream plenums of cylindrical shape. A convergent nozzle with a conical spine is placed at the downstream plenum end; this allows to adjust the outlet section to a well defined choke condition (according to the operating condition) and thus fixing the mass flow rate. Heat shield and dome are also present. The dome is not reproduced as a drilled plate, but is replaced by a porous domain with a calibrated momentum source: in such way it is possible to gain the correct air split between the injection system and the dome itself.

![FIGURE 5: ONERA TEST RIG](image)

![FIGURE 6: COMPLETE COMBUSTOR](image)

Figure 6 shows the good agreement between calculated and measured gas temperature, NOx and FAR profiles for the operating point A and B. All the values are evaluated on a transversal plane located 0.23 m downstream the dome. Table 2 summarizes the averaged quantity computed over such plane. The results are reported in non-dimensional form (reference level is the averaged experimental value, that is set to 1). The overall agreement with measurements is satisfactory for temperature and FAR profiles. At high pressure level (Operating Point B) it is immediately clear that NOx emissions are largely underpredicted. In principle, we can reach good accuracy in emission prediction through detailed chemical kinetics. This approach is considered the most realistic combustion mechanism in CFD, but, on the other hand, three problems arise:
large number of intermediate species (in the case of aero engine fuel, as JetA, such number is of the order of $10^3$);

- wide range of chemicals timescales (fast timescale for radical reactions, slow timescale for CO oxidation and NO\textsubscript{X} formation);

- efficient numerical methods are required to solve this numerically stiff set of equations.

The first two points can be summarized in a library in order to be used as input for the CFD evaluation. Since this library is not available, a fast chemistry approximation is used (as shown in the followings). This approach is suitable for fast combustion (mixing controlled) and gives good results for major species involved in global reactions. For this reason, ANSYS CFX is basically inadequate in the evaluation of intermediate products at high pressure levels. Anyway, it is possible to correct the reaction rate coefficients to follow the pressure dependency, but the results improvement is not appreciable.

An alternative approach is the evaluation of pollutant formation through post-processing considerations. In this manner, pollutants are solved with frozen velocity, turbulence, and composition field and radicals such as H and O needed in pollutant formation are reconstructed with assumptions. This method is then useful for qualitative considerations about how the device will work.

<table>
<thead>
<tr>
<th>Averaged Quantity</th>
<th>CFD</th>
<th>Averaged Quantity</th>
<th>CFD</th>
</tr>
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<tbody>
<tr>
<td>Temperature</td>
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<td>Temperature</td>
<td>0.9992</td>
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<tr>
<td>NO\textsubscript{X} emissions</td>
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<td>NO\textsubscript{X} emissions</td>
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<tr>
<td>FAR</td>
<td>1.0197</td>
<td>FAR</td>
<td>0.9999</td>
</tr>
</tbody>
</table>

Operating Point A Operating Point B

**TABLE 2: REACTIVE TEST RIG – CFD RESULTS VS. EXPERIMENTAL MEASUREMENTS – AVERAGED VALUES**

2. Application of all the assumed and tuned models and parameters developed in the previous stage to the single annular combustor model ⇒ the goal of this stage is to supply an estimation of the behaviour of the combustor in reactive frame. The details of this work phase are described in the followings.

**FIGURE 6: REACTIVE TEST RIG - CFD RESULTS VS. EXPERIMENTAL MEASUREMENTS**

**REACTIVE STUDY OF THE SINGLE ANNULAR COMBUSTOR**

**Layout**

The single annular combustor has been evaluated in this work phase in a reactive frame so as to estimate air split, temperature and pressure fields and emission levels. The results of the numerical simulations are useful to
have a complete comprehension about how the device works in reactive frame before its production.

The computational domain consists of a 20° sector of the single annular combustor (Figure 7 and Figure 8). Two plenums downstream inner and outer bleed holes are considered to stabilize the boundary conditions and to have a free flow through the bleed holes (not imposed). Dome and liners drilled plates are not explicitly reproduced here in order to reduce the model complexity. They are replaced by equivalent inlet and outlet boundary conditions. The CFD solver imposes a uniform flow field from the inlet boundary, but this is not true for the outlet boundary because it depends on the surrounding pressure and velocity field. Then, liners are split into several regions to assure the mass continuity through each region. The correct air split is detected through pressure drop considerations carried out by a preliminary run. The computational grid, shown in Figure 9, consists of about 12 millions elements.

Two different operating conditions have been considered:

1. Total pressure feeding 22.7 bar
   ⇒ this correspond to the Operating Point B for the tubular test rig evaluation ⇒ Operating condition 1

2. Total pressure feeding 33.46 bar
   ⇒ Take-Off Cycle ⇒ Operating condition 2

<table>
<thead>
<tr>
<th>Operating Condition</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Total Pressure [bar]</td>
<td>22.7</td>
<td>33.46</td>
</tr>
<tr>
<td>Inlet Temperature [K]</td>
<td>820</td>
<td>840</td>
</tr>
<tr>
<td>Pilot/Total Fuel Ratio</td>
<td>15%</td>
<td>10%</td>
</tr>
</tbody>
</table>

TABLE 3: OPERATING CONDITIONS

CFD: models and settings

The employed CFD software is ANSYS CFX. It is based on finite volume method and uses a coupled treatment to solve the linear set of equations that arise by applying such technique. Since the attention is primarily focused on the investigation of the average behaviour of the device, the flow is simulated as steady state.

A continuous gas phase (gas mixture) and a dispersed liquid phase (fuel) are considered in the computational domain. The fluids are mixed on a macroscopic scale and interact with each other by means of interfacial forces and heat and mass transfer across the phase interfaces. In this case, it is necessary to solve for different velocity and temperature fields, etc., for each fluid (multiphase flow simulation).

The Particle Transport Model in ANSYS CFX is capable of modelling dispersed phases (particles) which are discretely distributed in a continuous phase. The modelling involves the separate calculation of each phase with source terms generated to account for the effects of the particles on the continuous phase. A Lagrangian transport model is used for the dispersed phase and all continuous phases use the Eulerian model.
All the following considerations about gas phase and particles/liquid phase models have to be considered as an evolution of a pre-existent procedure. Such methodology has been developed by the collaboration between EnginSoft and Avio and it has been widely employed up to now. An important opportunity is given in the frame of NEWAC research project to develop a new procedure setting up new models implemented in the very last releases of the CFD code. The first improvement regards the turbulence model: a comparison between the standard k-ε model and the ω-based Shear Stress Transport (SST) model has been performed. The latter guarantees a better definition of the onset and amount of flow separation because of a different definition of the turbulent shear stress, but, on the other hand, convergence becomes slightly tricky. As will be explained in the following paragraphs, fuel film formation is involved in this problem. Currently there is no method in ANSYS CFX for accurately simulating this type of phenomena. However, setting a small positive value for the perpendicular coefficient of restitution can be useful to avoid particles that bounce off the injection system walls. In such way, no more combustion is observed within the injection system due to unrealistic bounced evaporated particles.

Another aspect that has been investigated is the interaction between particles and air streams. In the old procedure the droplets dimension distribution is directly set taking into account both primary and secondary breakup processes (empirical formulas from literature). Several computational models have been developed and validated in the meanwhile, so a secondary breakup process is activated in the new methodology.

**Gas mixture (gas phase)**

Reynolds Averaged Navier-Stokes (RANS) equations are computed to solve the continuous gas phase flow field. The total energy heat transfer model is selected for the gas phase flow because it includes kinetic energy and compressibility effects (the Mach number surely exceeds 0.3 somewhere in the domain). The adopted turbulence model is the SST with automatic near-wall treatment [3].

**Fuel (liquid phase)**

Material

The considered fuel is JetA. This is a type of aviation fuel designed for use in aircraft powered by gas-turbine engines. All the properties are drawn from ANSYS CFX material database.

Momentum Transfer

Fully coupled fuel particles exchange momentum with the continuous gas phase, allowing the gas flow to affect the particles, and the particles to affect the gas flow.

**Gas mixture (gas phase)**

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**Heat Transfer**

The rate of change of particle temperature is governed by two physical processes: convective heat transfer and latent heat transfer associated with mass transfer. The convective heat transfer \( Q'_c \) is given by:

\[
Q'_c = \pi d^2 \lambda \frac{\partial T}{\partial r} \quad \zeta \quad \frac{e^{-\zeta}}{1 - e^{-\zeta}}
\]

where \( d \) is the particle diameter, \( \lambda \) is the thermal conductivity of the fluid, \( T_c \) is the fluid temperature, \( T \) is the particle temperature, and \( \zeta \) is the Nusselt number, expressed by Ranz-Marrshall correlation for a sphere:

\[
Nu = 2 + 0.6 \Re^{0.5} \Pr^{1/3}
\]

Equation 1

In multiphase reactions cases like this, the convective heat transfer has a blowing correction based on the rate of mass transfer from the particle:

\[
Q_c = Q'_c \zeta = \frac{\frac{dm}{dt}}{\pi d \lambda Nu}
\]

where \( \zeta \) is given by:

\[
\zeta = C_p \frac{\frac{dm}{dt}}{\pi d \lambda Nu}
\]

\( \frac{dm}{dt} \) is the total mass transfer rate of the particle.

The heat transfer associated with mass transfer \( Q_M \) is given by the relation:

\[
Q_M = \frac{dm}{dt} V
\]

The latent heat of vaporization \( V \) is temperature dependent, and is obtained directly from the material data set for the liquid in the particle and its vapor.

The temperature variation for the particle is then:

\[
mC_p \frac{dT}{dt} = Q_c + Q_M
\]

Mass Transfer

The mass transfer from liquid drops is modeled with the Liquid Evaporation Model. This option is used to model evaporation of a liquid species in particles to the respective gas phase species in the continuous phase (one component mass transfer). The model uses two mass transfer correlations depending on whether the droplet is above or below the boiling point. This is determined through the Antoine equation:

\[
P_{vap} = P_{ref} \exp \left( A - \frac{B}{T - C} \right)
\]

Equation 2
where \( A, B \) and \( C \) are taken from the literature. Specifically, \( A = 23.3, B = 5600 \text{K} \) and \( C = 25 \text{K} \). The particle is boiling if the vapor pressure \( P_{\text{vap}} \) is greater than the gaseous pressure \( P_{\text{ref}} \).

When the particle is above the boiling point, the mass transfer is determined by the convective heat transfer:

\[
\frac{dm}{dt} = \frac{Q_C}{V}
\]

When the particle is below the boiling point, the mass transfer is given by the formula:

\[
\frac{dm}{dt} = -\pi d_p \rho_f D_f Sh \frac{W_C}{W_G} \log \left( \frac{1 - X \ast}{1 - X_G} \right)
\]

where \( \rho_D \) is the dynamic diffusivity of the mass fraction in the continuum, \( W_C \) and \( W_G \) are the molecular weights of the vapor and the mixture in the continuous phase, \( X_G \) is the molar fraction in the gas phase and \( X \ast \) is the equilibrium mole fraction at the droplet surface, defined as \( P_{\text{vap}} \) divided by the pressure in the continuous phase. \( Sh \) is the Sherwood number, given by:

\[
Sh = 2 + 0.6 \text{Re}^{0.5} \left( \frac{\mu}{\rho D} \right)^{3/5}
\]  
Equation 3

A modification parameter named Light Oil is also enabled to control the physical properties used in calculating the heat and mass transfer from the droplet: such option fixes the physical parameters used in the Reynolds number, the Nusselt number (Equation 1) and the Sherwood number (Equation 3) on the gas assumed to be in the boundary layer of the droplet. This, in turn, depends upon the Antoine equation (see Equation 2; i.e., if the drop is boiling, the gas in the boundary layer is all volatiles). In the other extreme, the gas in the boundary layer consists entirely of the local gas mixture.

Particle Injection

The fuel staging process consists of a double fuel injection (see Figure 10): the pilot line, which fuel injector is a conventional pressure atomizer, and the main line. The fuel provided by the main line flows into the primary swirler passage through small ducts; the effect of the incoming air stream is to create a film on the injection system walls and drag such film towards the lip of the injection system. Here, the air streams coming from primary and secondary swirler vanes interact causing a stripping and finally a fine atomization of the film. In this activity the complexity of the main line is not reproduced: the effects of the film formation and the relative atomization at the lip are replaced by the imposition of an equivalent second particles injection region at the lip (annular region). The particle diameter obeys the Rosin-Rammler distribution for both the injection regions. Moreover, a particle secondary break-up model is activated and the Taylor Analogy Breakup (TAB) model is selected. It is assumed that the droplet distortion can be described as a one-dimensional, forced, damped, harmonic oscillation similar to the one of a spring-mass system. In the TAB model, the droplet deformation is expressed by the dimensionless deformation \( \tilde{y} \). Breakup only occurs if the particle distortion \( \tilde{y} \) exceeds unity, which means that the deviation of the particle equator from its equilibrium position has become larger than half the droplet radius [4],[5].

![FIGURE 10: INJECTION SCHEME](image-url)

Combustion

In such reactive problem the combined Finite Rate Chemistry/Eddy Dissipation Model (FRC/EDM) is set: the reaction rates are first computed for each model separately and then the minimum of the two is used. This procedure is applied for each reaction step separately, so while the rate for one step may be limited by the chemical kinetics, some other step might be limited by turbulent mixing at the same time and physical location. The combined model is valid for a wide range of configurations, provided the flow is turbulent. In particular, the model is valid many reactions which range from low to high Damköhler numbers (chemistry slow/fast compared to turbulent time scale). The combustion is modelled by two-step kinetic scheme, as follows:
\[ C_{12}H_{23} + \frac{47}{4} O_2 + \frac{23}{2} H_2 O \rightarrow 12 CO + \frac{23}{2} H_2 O \]

\[ R_1 = 2.08e^{14} \cdot e^{-2700[K]/T} \left[ \frac{m^{1.5}}{mol^{0.5} \cdot s} \right] \]

\[ CO + \frac{1}{2} O_2 \rightarrow CO_2 \]

\[ R_2 = 2.22e^{7} \cdot e^{-1250[K]/T} \left[ \frac{m^3}{mol \cdot s} \right] \]

Obviously, the NO formation model is considered in order to take into account NO\(_x\) emissions. The thermal NO mechanism is a predominant source of NO\(_x\) in gas flames at temperatures above 1800 K. The NO is formed from the combination of free radical O and N species, which are in abundance at high temperatures. The two-step mechanism (Zeldovich mechanism), is assumed to dominate the process:

\[ O + N_2 \rightarrow NO + N \]  
**Reaction 1**

\[ R_3 = (1.8 \cdot 10^{11}[m^3 kmol^{-1} s^{-1}])e^{(-38370[K]/T)} \cdot [O]^{1.0} \cdot [N_2]^{1.0} \]

\[ N + O_2 \rightarrow NO + O \]  
**Reaction 2**

\[ R_4 = (6.4 \cdot 10^9[m^3 kmol^{-1} s^{-1}])e^{(-3164[K]/T)} \cdot [N]^{1.0} \cdot [O_2]^{1.0} \]

In sub or near stoichiometric conditions, a third reaction may be important:

\[ OH + N \rightarrow NO + H \]  
**Reaction 3**

\[ v_3 = 3.0 \cdot 10^{14}[m^3 kmol^{-1} s^{-1}] \cdot [OH]^{1.0} \cdot [N]^{1.0} \]

When this step is included with the first two, it is referred to as the extended Zeldovich mechanism [5]. The rates of each of these reactions are proposed in [6]. The first step tends to be rate limiting, producing both an NO and N radical species. The N radical is assumed to be oxidized by Reaction 2 in the Zeldovich mechanism and also by Reaction 3 in the extended Zeldovich mechanism. Either way, these second oxidation reactions are assumed to be fast and if Reaction 1 occurs, then two NO molecules will be formed. The thermal NO formation is therefore related to the rate of Reaction 1 as follows:

\[ S_{NO, thermal} = W_{NO} R_{NO, thermal} [O][N_2] \]

\[ R_{NO, thermal} = 2R_1 \] and \( W_{NO} \) denotes the molecular mass of NO. Thus, if the molar concentrations \([O]\) and \([N_2]\) of O radicals and N\(_2\) are known, the thermal NO mechanism can be calculated. When using the combined FRC/EDM model, O radical concentrations usually are not known directly but must be derived from other quantities. Here, the O radical concentration \([O]\) is estimated from the molecular oxygen dissociation (Westenberg, 1975):

\[ \frac{1}{2} O_2 \leftrightarrow O \]

\[ [O] = 12567[kmol^{0.5} m^{-1.5} K^{-0.5}] \cdot T^{-0.5} \cdot e^{-\left[31096[K]/T\right]} \cdot [O_2]^{0.5} \]  
**Equation 5**

Equation 5 is then substituted in Equation 4; moreover, to adjust such model to high pressure condition, the pre-exponential factor of first step, which tend to be rate limiting, is increased. Then, the thermal NO formation rate is:

\[ R_{NO, thermal} = 5.164 \cdot 10^{11}[m^3 kmol^{-1} s^{-1}] \cdot 12567[kmol^{0.5} m^{-1.5} K^{-0.5}] \cdot \cdot e^{-\left[38370[G]/T\right]} \cdot 12567[kmol^{0.5} m^{-1.5} K^{-0.5}] \cdot \cdot e^{-\left[31096[K]/T\right]} \cdot [O_2]^{0.5} \]

**Computational considerations**

The employed advection scheme is the Specify Blend. Values between 0.0 and 1.0 blend first and second order differencing, with increased accuracy and reduced robustness as value 1.0 has approached. At lower values, excessive diffusivity can occur. At the higher values, overshoots and undershoots can appear. Therefore, a good compromise has been found with a value of 0.7.

Double precision accuracy is also needed to permit more accurate numerical mathematical operations. In fact, the computational domain involves a wide variation of all the variables because of combustion process, especially between periodic interfaces.

Convergence is verified by checking the size of the RMS residuals (local imbalance of each conservative control volume equation), as well as the overall flow balances (overall conservation).

<table>
<thead>
<tr>
<th>RMS mass residuals</th>
<th>&lt; 1e-6</th>
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<tbody>
<tr>
<td>RMS momentum residuals</td>
<td>&lt; 1e-4</td>
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<td>RMS energy residuals</td>
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<td>RMS turbulence residuals</td>
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<tr>
<td>Imbalance</td>
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</table>

**TABLE 4: CONVERGENCE DETAILS**

All calculations have been performed on a Linux cluster on which Intel(R) Xeon(R) X5355 (quadcore, 64 bit, 2.66GHz) CPUs are installed. In order to save time, 32 partitions have been considered. In such way the total elapsed CPU time to complete 1500 iterations is about 36 hours.

**Results**

The results of the CFD simulations about the complete annular combustor in reactive frame are described in Figure 11 in terms of velocity field, emissions and turbulent kinetic energy. All the results reported are referred to the simulations performed with the SST turbulence model and the values are expressed in non
dimensional form (reference level is maximum value in the quantity field considered).

A comparison between the two considered operating points is shown. The main variations in the behaviour of the device are principally due to different pressure levels: the higher is the pressure, the higher is the combustion rate. Moreover, the turbulent kinetic energy is also interesting because, according to the combined Finite Rate Chemistry/Eddy Dissipation model, it participates in the activation of the combustion process.

The layout here discussed is the best among all the considered ones in terms of size, position and stability of the recirculation zone. The resulting pressure levels in the combustion chamber satisfy the requirement for the combustion process.

The aerodynamic shape of the fuel tube keel allows to reduce its wake in the outer annulus; this, in turn, allows a correct air split distribution for outer bleed holes and dilution holes.

Unfortunately, a comparison between CFD results and measurements is not available today, since experimental test are scheduled only for Q1/Q2 2010.

**CONCLUSIONS**

The Lean-Burn innovative injection system of the NEWAC Low-NOx single annular combustor has been considered in this activity.

The injection system has been widely tested in reactive frame by ONERA Laboratory on a tubular test rig. The experimental data have been referenced to validate the CFD numerical models for the flow field, i.e. boundary conditions, advection scheme, multi-phase and particle transport, and combustion, i.e. kinetic scheme. The numerical procedure has been applied to evaluate the performance of the complete single annular combustor, so as to estimate air split, temperature and pressure fields and emission levels before its production. An accurate design of the cowl allow to reach the correct working of the lean combustor, demonstrating the validity of the original principle of the injection system.

Looking at the CFD results, we could be quite confident for the prediction of the temperature field in the complete annular combustor. Computed emissions are not quantitatively satisfactory at relatively high pressure level (large under-prediction due to the lack in the ANSYS CFX code in the evaluation of intermediate products for such conditions). However, these data could be useful for qualitative considerations about how the device will work (post-processing considerations).

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**NOMENCLATURE**

ACARE: Advisory Council for Aeronautical Research in Europe
ANTLE: Affordable Near-Term Low Emissions
CAEP: Committee for Aviation Environment Protection
CAE: Computer-Aided Engineering
CFD: Computational Fluid Dynamics
CLEAN: Component vaLidator for Environmentally-friendly Aero-eNgine
EEFAE: Efficient, Environmentally Friendly Aero-Engine
FAR: Fuel Air Ratio
NEWAC: NEW Aero engine Core concept
OPR: Overall Pressure Ratio
SP: Sub-project
VITAL: enVironmenTALy Friendly Aero Engine

**REFERENCES**

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FIGURE 11: CFD RESULTS COMPARISON BETWEEN 2 OPERATING CONDITIONS