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Advanced Simulation of Aeronautical Combustors

The development of new aeronautical combustor concepts relies on the best possible knowledge of combustion phenomena, such as ignition and extinction, flame structure, combustion instabilities or pollutant emissions. Numerical simulation, and in particular the Large Eddy Simulation approach, is a powerful tool to understand, predict and control the coupled physics involved in turbulent combustion in both academic and applied configurations. Thanks to reliable physical models, accurate numerical methods and high efficiency on massively parallel computers, numerical simulation is now able to produce robust and reliable solutions in complex geometries, taking into account all technological and physical effects. Today, it is a research tool that contributes to improving our knowledge of turbulent reacting flows and in particular the interaction between turbulence and combustion chemistry. It is also an efficient tool for the design of aeronautical combustors, guiding test benches and possibly reducing their number.

Introduction

In recent years, numerical simulation has gained considerable importance in the understanding and prediction of combustion phenomena in both academic and applied configurations. It is a challenging domain that requires suitable descriptions of the turbulent flow and the chemistry, as well as their strong interaction and other coupled physics such as spray injection, heat transfer and acoustic resonances with the system modes, etc. The numerical simulation of turbulent reacting flows relies on the accurate modeling of the underlying physics, which has been developed by a large community in the past 50 years and is still the focus of intense research [1]. Its capabilities to address large, transient and multi-physics problems have been promoted by the development of High Performance Computing (HPC), that has considerably improved the fidelity of the results and opened new fields of research [2]. HPC also plays a key role in the implementation of numerical simulation in the industrial context, making it an efficient design tool capable of taking into account complex geometries with an increasing number of technological details.

Models and numerics for advanced simulation of aeronautical combustors

In the field of turbulent - inert or reacting - flows, numerical simulation techniques can be classified depending on their level of accuracy. Direct Numerical Simulation (DNS) consists in solving the turbulent flow equations without any modeling, which implies that the full range of turbulent scales must be resolved. This requires the number of discretization points N to increase as $Re^{3/4}$ in each direction, so that the total number of nodes in the grid increases as $Re^{9/4}$, where $Re = U L/\nu$ is the Reynolds number. In reacting flows, the very thin reaction zone requires even smaller grid cells. In contrast, the Reynolds-Averaged Navier Stokes (RANS) relies on the statistical moments (mean and rms) of the flow, solving ensemble-averaged flow equations with various closures for the turbulent Reynolds stresses and fluxes, and dropping out the description of the various scales of the turbulent flow. Due to their computational cost, DNS calculations are exclusively dedicated to academic, simple-geometry, small-scale configurations with a moderate Reynolds number, with the aim of accurately describing the complex structure of turbulence and its interaction with a flame front. On the other hand, the fast RANS approaches are most suitable for industrial application, although their fidelity and capacity to represent complex non-linear physics are limited. It is known, for example, that RANS methods do not provide an adequate representation of rotating flows of the type induced by swirl injectors. In recent years, the Large Eddy Simulation (LES) technique has emerged as a good compromise between DNS and RANS, keeping high accuracy and fidelity at a reasonable CPU cost. This is achieved by applying a low-pass spatial filter to the flow equations, eliminating the smaller scales that are easily modeled. LES therefore still solves for physical variables, keeping their time and space scales down to the filter cut-off scale. Contrary to DNS, where high-order numerical schemes impose simple geometries, LES may rely on 3rd or even 2nd order non-dissipative schemes, which are still useable at a reasonable CPU cost in complex geometries. Lower order schemes, which are commonly used in RANS, are however not appropriate for LES where the subgrid scale turbulent viscosity is much smaller than in RANS.

Combustion chemistry must also be described, since it drives all flame characteristics and behaviors of interest within the framework of burner design: ignition and extinction, flame structure, burnt gas state, pollutant emissions, etc., are all strongly dependent on chemistry and of primary importance for the burner performances. For standard kerosene or jet fuels, combustion chemistry involves hundreds of chemical species and thousands of reactions, which strongly raise the CPU cost if directly computed. Many approaches exist to account for complex fuel chemistry and its interaction with the turbulent flow in the thin flame regime, which corresponds to the situation prevailing in engines [3, 4, 5, 6, 7]. One strategy is then to pretabulate the detailed chemistry flame structure as a function of one or two parameters (typically the progress variable and the mixture fraction), later introduced into the simulation via the Probability Density Function (PDF) of the tabulation parameters, or via the Flame Surface Density concept. Another strategy is to reduce the chemical scheme to a limited number of species and reactions, still guaranteeing the correct flame characteristics and behaviors. The flame structure can then be computed directly, modeling its interaction with turbulence through an additional model, such as the Thickened Flame model in the LES context (TFLES). Global chemical schemes, reduced down to 1 to 4 steps, are usually built with a fitting procedure, and are valid only under the fitting range conditions. More sophisticated methods are used to analytically derive reduced schemes [8], involving 10 to 25 species depending on the fuel, which reflect the main chemical paths and reproduce the correct system behavior under a wide range of conditions.

Ignition and extinction

From one sector to full burner ignition

Ignition constitutes a critical phase in aerospace propulsion. It must be completed in a safe and reliable way, i.e., always leading to a stabilized flame, while producing a minimum pressure peak, even under unfavorable conditions at high altitude, where rapid relight in case of accidental extinction of the combustor is required for engine certification. New combustion technologies currently developed to reduce pollutant emissions, make the ignition process even more critical.

The experimental characterization of ignition has been extensively studied on single burner ignition problems. One of the key issues is to predict the survival of the generated flame kernel in the turbulent flow field. Indeed, depending on the local flow conditions that are encountered by the kernel, it can either develop towards a turbulent flame or extinguish, leading to a measurable probability of ignition. Computing a full probability map numerically demands important computational resources, since many ignition events must be simulated. This has been achieved in recent work [9], where a good agreement between the numerical and experimental probability maps has quantitatively validated the predictability of LES. Such simulations also enabled a better physical understanding of the stochasticity of the ignition process to be achieved and a low-order predictive model that can be used repeatedly at the industrial design stage [10, 11] could be provided.

Applying LES to the full ignition process has been the next important challenge. Following the pioneering work of Boileau et al [6], Barré et al [12] performed a joint analysis of experiments and numerical simulation of ignition in a gaseous non-premixed multi-injectors burner, in order to study the effects of spacing between injectors on the ignition process and the mechanisms driving the flame propagation from burner to burner. More recently, a novel experimental device named MICCA [13] has been simulated [14, 15] with the AVBP solver, a code jointly developed by CERFACS and IFPEN [16]. This system comprises 16 swirling injectors in an annular geometry allowing full optical access to the flame. It is fed with a lean mixture of air and propane while a single spark igniter initiates the flame. In the simulation, the turbulent combustion is described with either the Filtered Tabulated Chemistry LES model F-TACLES [7] or the TFLES model [17]. With a mesh of 310 million tetrahedra, the simulation required 1.5 million CPU hours on TGCC-Curie thin nodes and was efficiently run on 6144 CPU cores. For both F-TACLES and TFLES models, numerical results closely match experimental data, as illustrated in Fig. 1. The flame brush at the largest scales is similar to that observed experimentally; the instantaneous flame configurations resemble those recorded by the camera. Transit times from one injector to the next match the measured ones, and the duration of the light-round of the order of 50 ms is also correctly predicted.

Extinction limits

The design of gas turbine burners requires the characterization of their operability, and in particular their lean blow-off limits (LBO) in terms of Fuel-Air Ratio (FAR). Flame extinction is however a complex transient process, driven by the two-phase flow, flame structure and their response to varying operating conditions. Experimentally, LBO is usually characterized by reducing the FAR gradually until extinction.

The same methodology has been applied to predict the LBO limit with LES for a variety of SAFRAN combustors and operating conditions (pressure and temperature). Simulations were performed with the AVBP solver, using the TFLES model [17] combined with a two-step kinetic mechanism for the kerosene chemistry [18]. For confidentiality reasons, extinction limits presented in Fig. 2 are normalized by the FAR at take-off power. A very good agreement between numerical and experimental results is obtained for the FAR extinction limit of real burners. In such a diagram, overall absolute errors are lower than $\pm$ 2 thousandths. The various configurations and operating conditions are also correctly ranked, validating the use of LES for LBO operability issues.

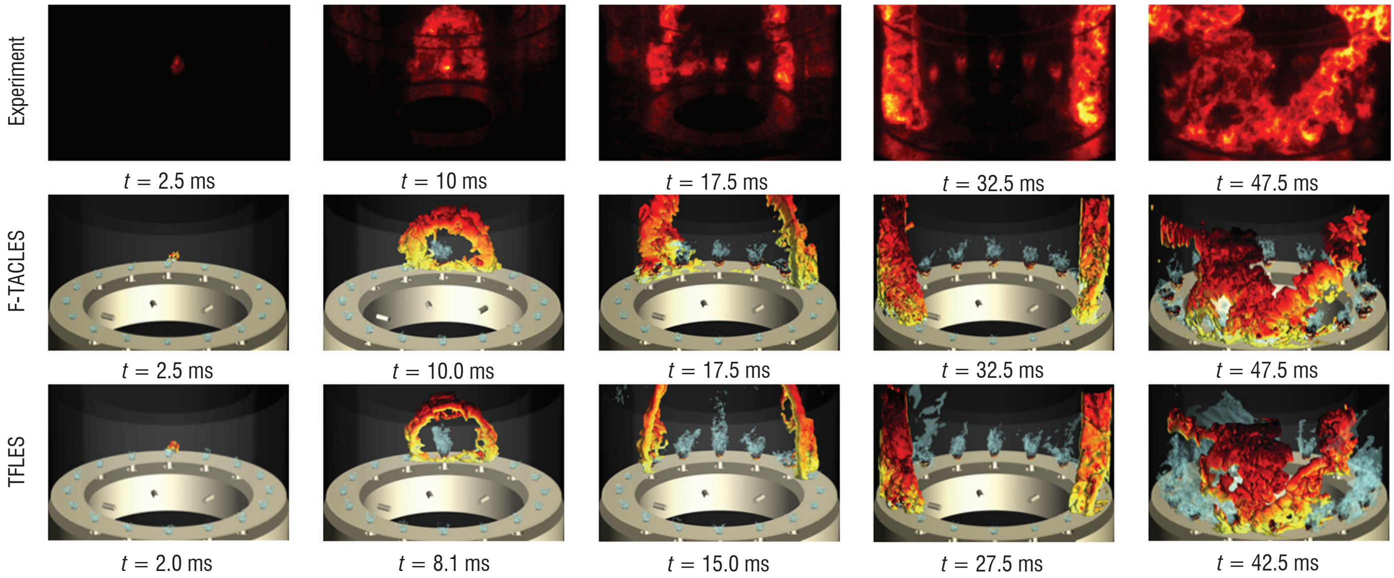

Figure 1 - Five instants in an ignition sequence of the MICCA chamber. Top row: Experimental views showing light intensity emitted by the fame during the light-round process, and represented in false colors to improve visualization. Middle and bottom rows: Respectively F-TACLES and TFLES simulations. Flame fronts are represented by an isosurface of progress variable c=0.9 for F-TACLES, corresponding to an isosurface of temperature T= 1781 K for TFLES. Both are colored by axial velocity levels (light yellow: -30ms-1; black: +15ms^{-1}). Blue isosurfaces correspond to the velocity field U = 25ms^{-1} (from [15]).

Combustor performances

Temperature distribution at the combustor exit

One of the uses of LES within the framework of combustion chamber design concerns the prediction of the temperature level and its spatial distribution at the combustor exit which is an input for high pressure turbine designers. Figure 3 shows a typical example of a straight-through combustion chamber geometry from SAFRAN along with the associated exit plane position.

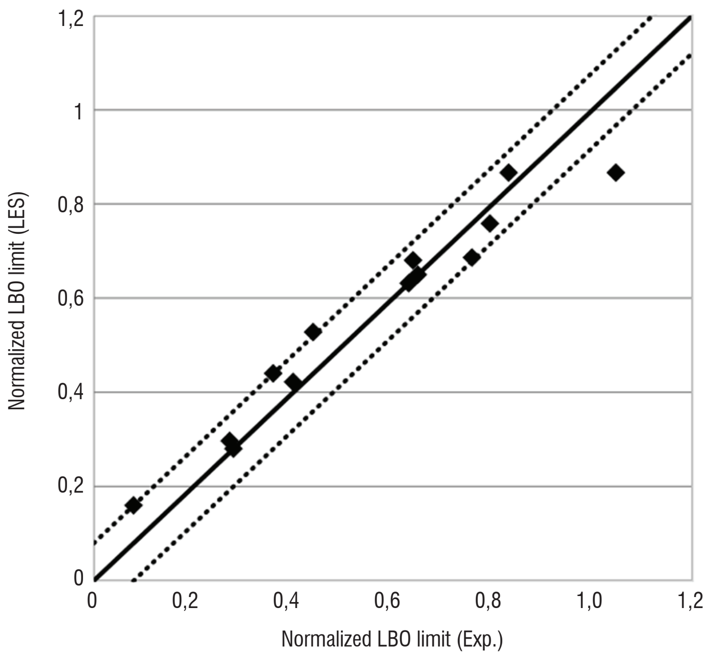

Figure 2 - LBO limit prediction (LES) vs. experimental data for a set of SAFRAN combustors under various operating conditions. Values are normalized by the fuel-air ratio at take-off power. Dotted lines correspond to the absolute error zone of ± 2 thousandths.

For analysis and exchange of information with the turbine designers, a dimensionless temperature 1D profile (azimuthal average) is usually extracted from the LES field, leading to the so-called RTDF profile. Several LES calculations were carried out on about ten combustors, using exactly the same simulation set-up in terms of models and numerics. In Fig. 4, results are compared to measurements at various radii across the vane. They are normalized for confidentiality reasons by the maximum of the RTDF profile. There is a relatively good agreement between numerical results and measurements in the hot part of the vane, since the error lies within the ± 2 point tolerance zone (not shown).

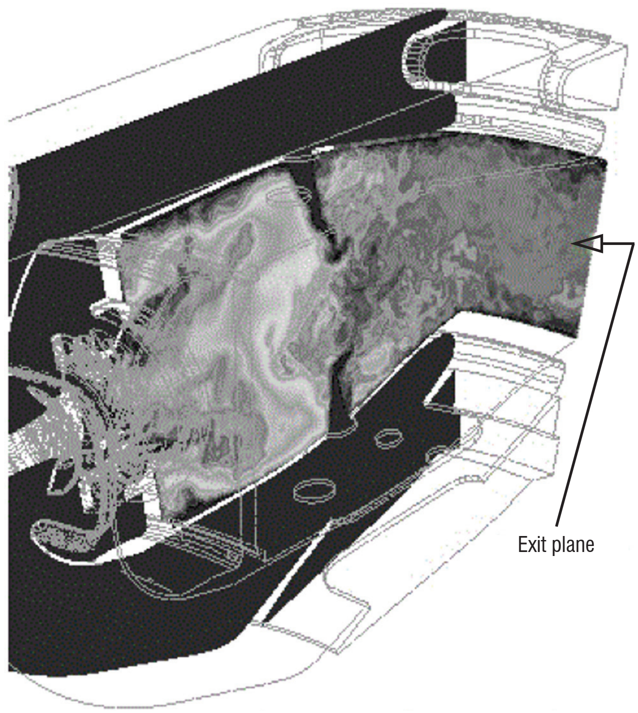

Figure 3 - Example of a straight-through combustion chamber and its exit plane location.

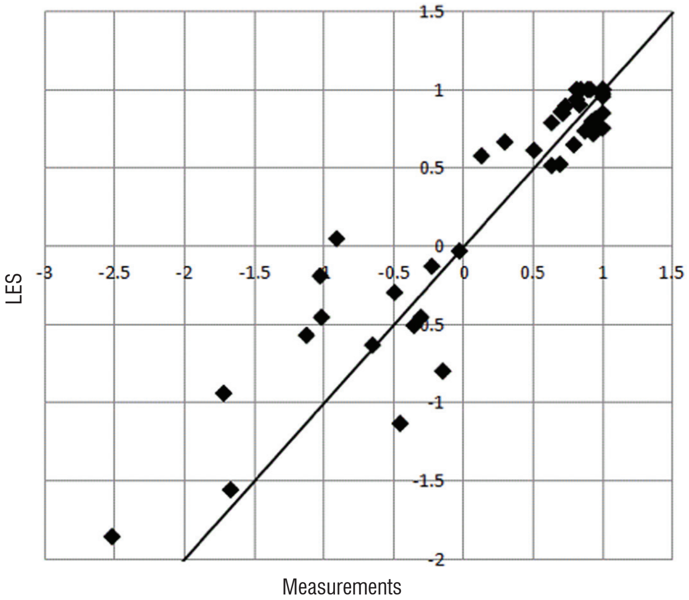

Figure 4 - Dimensionless temperature (RTDF) at various radii for a set of SAFRAN combustors. RTFD values are normalized by the maximum of the 1D profile.

A monotonic trend is also observed confirming that the hottest zones are well positioned. The largest differences are found near the walls, where temperature levels are not well captured. At this point, it should be noticed that effusion cooling at the combustor walls was described with a homogeneous approach [19], which is suspected to underestimate mixing in the liner vicinity. Improvement of the near wall behavior is expected with heterogeneous descriptions such as the one recently developed by CERFACS and SAFRAN TURBOMECA [20].

Combustion instabilities

Combustion instabilities are a major concern in the design process of industrial combustion chambers. They are characterized by strong pressure and heat release oscillations in the flame tube and can alter the integrity of the system. Compressible LES is an appropriate tool to study combustion instabilities, because it takes into account the main processes involved: flame dynamics, acoustics, turbulence and various dissipation mechanisms. LES of three industrial configurations from SAFRAN have been carried out for operating points featuring a strong acoustic response characterized by pressure oscillations at a particular frequency and amplitude. The acoustic mode appears naturally in the simulation after a transient phase, growing until it reaches a limit cycle. Comparisons between experimental and numerical frequencies are shown in Fig. 5 for the three combustion chambers. Two of them feature longitudinal acoustic modes that were obtained on a single sector of the combustion chamber [21, 22]. The third one features an azimuthal mode and can only be obtained by considering the full annular combustor [23].

The frequencies obtained in the simulations are quite close to those observed experimentally, showing that the acoustics and the combustion response are sufficiently well resolved. Some differences are observed for the amplitude, though the order of magnitude is correct. Current investigations rely on the complementary development of acoustic tools and reduced models to incorporate the action of the flame on the acoustic stability of an engine. In parallel, the question of the flame response to acoustic solicitations is naturally raised and the subject of dedicated LES-based studies [24].

Pollutants and soot

Prediction of NOx in aero-engines

Environmental constraints, and in particular Nitrogen oxides (NOx) and CO emissions, are also an important part of aeronautical burner design. NOx are mainly produced in a thermal pathway where both hot temperature and oxygen are present [25], complemented by a prompt pathway in the fuel oxidation layer of the flame front [26]. The time scale of the thermal NOx chemical pathway being far longer than that of kerosene oxidation in the flame front [27, 28], it requires dedicated modeling. Within the framework of tabulated chemistry models [29, 30], Pecquery et al recently proposed the NOMANI model (Nitrogen Oxide emission model with one-dimensional MANIfold) [31], which relies on two different progress variables to take into account both the thermal and prompt NOx pathways, as well as the dilution of the burnt gases by effusion holes after the primary zone of the combustor. In order to generate the 1D premixed laminar flames of the table for the

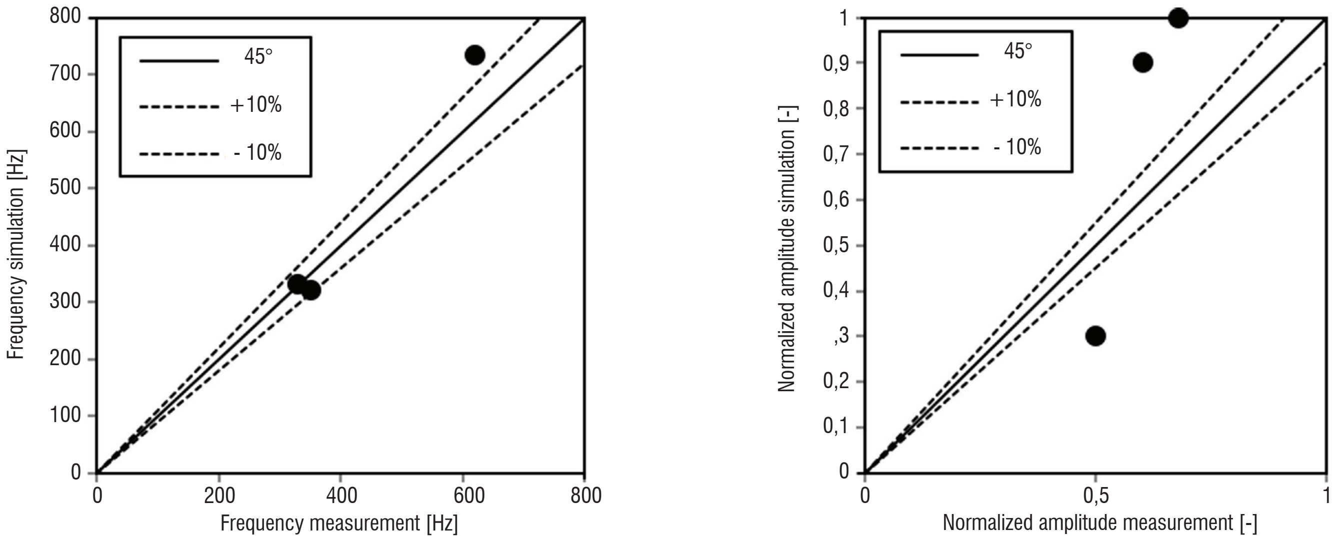

Figure 5 - Unstable modes for three different real scale combustors.
Comparaison between LES and experiments in terms of frequency (left) and normalized amplitude (right).

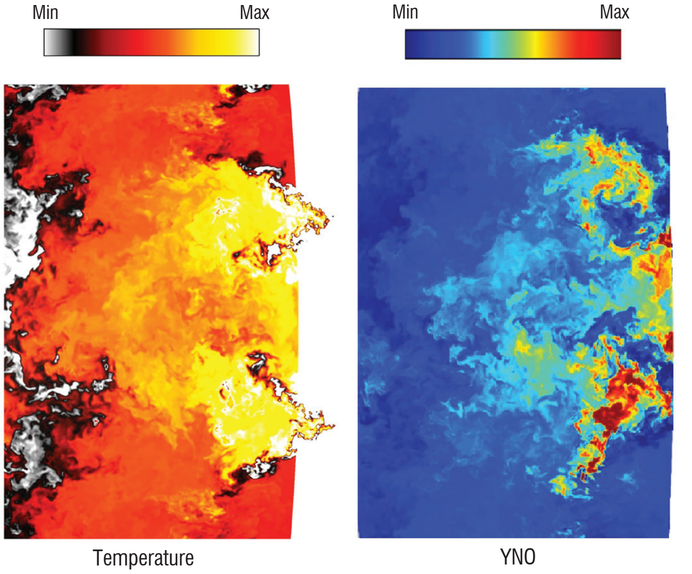

Figure 6 - Instantaneous fields of temperature and NO mass fraction at the center of the burner. Injection is on the right side.

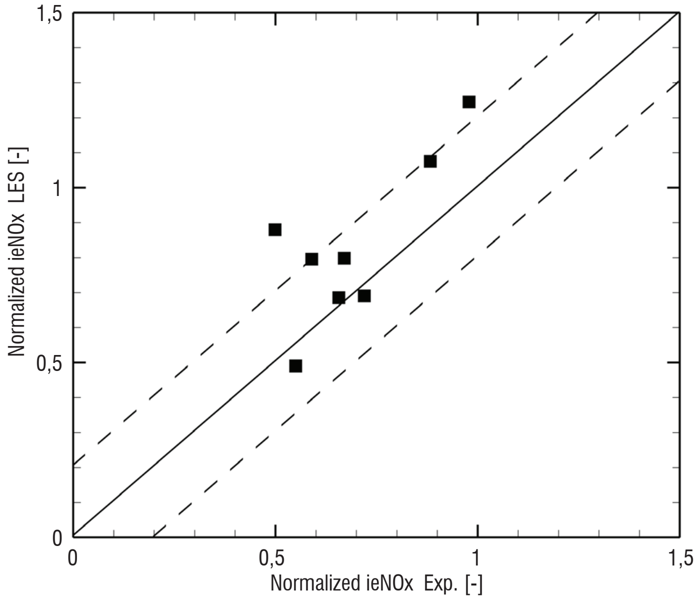

Figure 7 - LES normalized NOx emission index as a function of the experimental ones for various operating conditions and combustion chamber technologies.The dashed lines outline the experimental strong confidence zone.

full range of operating conditions of aeronautical burners in terms of pressure, inlet temperature and equivalence ratio, a parallel table generator based on the Cantera software [32] has been designed. The tool called MUTAGEN (MUlticore TAble GENerator) relies on pre-existing flame repositories, used as initial conditions to converge new flames, and allows look-up tables to be obtained, in the worst case within 2 to 3 hours on 16 cores for the reduced Luche mechanism [33, 34], which contains 92 species and 694 reactions.

The NOMANI model was implemented in the YALES2 solver developed at CORIA [35, 36]. The YALES2 code is dedicated to the LES of turbulent reactive flows on unstructured grids at low-Mach number. YALES2 has been specifically tailored for exploiting massively parallel computers and the handling of meshes with billions of cells [37]. The YALES2 code and the NOMANI model were recently applied at SAFRAN TURBOMECA to a low-NOx burner. These simulations count 380 million tetrahedra for a sector of two injectors and run on 2048 cores of the Airain machine at the TGCC center of the CEA. Instantaneous temperature and NO mass fraction fields at the center of the burner are represented in Fig. 6, illustrating the strong correlation between the two fields. In the primary zone, hot temperatures and high NO mass fractions appear in the same regions: in the central recirculation zone of each injection system and also to a less extent in the recirculation zones between the injection systems. The same methodology was applied to various operating conditions, combustion chambers and injector technologies at Safran. A reduced set of results is illustrated in Fig.7, where the numerical, normalized NOx emission indices are compared with experimental values. The results are consistent with the experimental data, and mostly within experimental uncertainties. These calculations pave the way for a better understanding of NO emissions in gas turbine combustors and the ability to optimize the air split in the burner for reduced NO production.

Soot

Soot participates in the energy balance in the production chamber, modifying the burnt gas temperature. It can cause a significant loss of efficiency of aeronautical combustors, due to soot deposits and wall deterioration. In addition, when emitted to the atmosphere, soot aggregates have a negative impact on health and the environment.

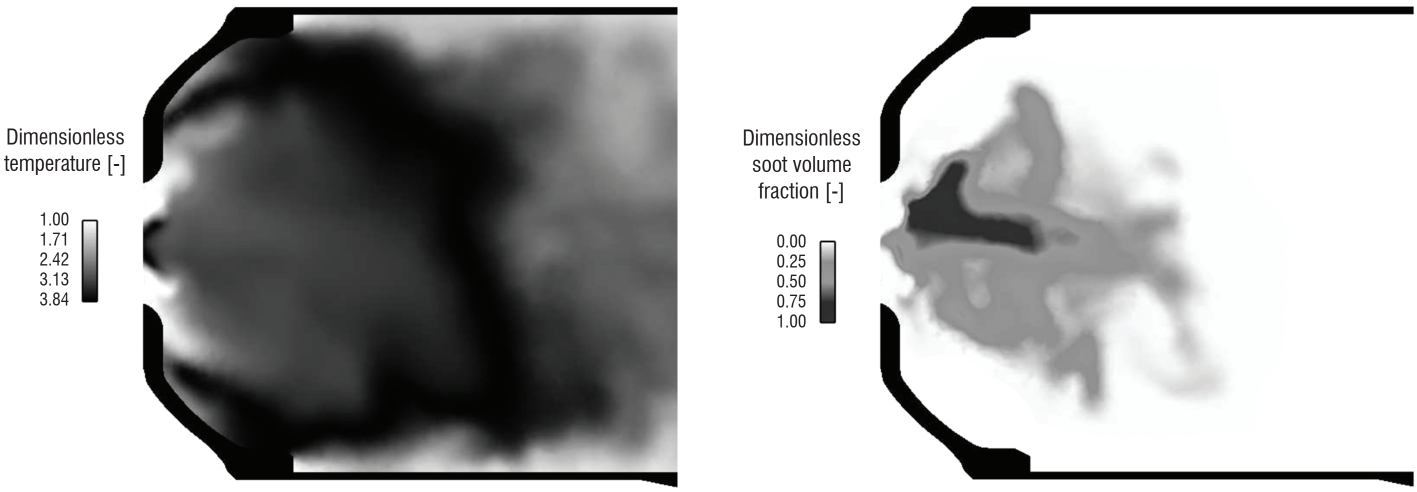

Figure 8 - Instantaneous dimensionless temperature and soot volume fraction fields in a SAFRAN TURBOMECA helicopter model combustor.

Soot production is the result of a complex heterogeneous chemical process, where gaseous precursors trigger the formation of solid particles that may aggregate and react on their surface. Like combustion, this chemical phenomenon is quite sensitive to turbulent transport and mixing, which makes soot highly intermittent and strongly dependent on the temporal and spatial evolution of the flow. Therefore, LES is the most adequate numerical method to investigate soot production in aircraft engines. To do so simplified soot models are used, and coupled to temperature and species fields, as well as thermal radiation.

Coupled LES-radiation simulations have been recently presented in [38, 39] to evaluate soot particles in a helicopter engine. The solid phase has been described by a phenomenological two-equation model [40], where acetylene is the only soot precursor and soot oxidation is due to OH and O2. A hybrid chemical description has been proposed by [38], combining a two-step global chemistry for the gas phase combustion [18] and a tabulated chemistry for the minor species involved in soot production but not present in the reduced chemistry. Finally, a Discrete Ordinates Method approach with optimized spectral models has been used to compute radiation [41]. It was shown that soot is produced and grows in the rich zones of the primary premixed flame, and is then consumed in a secondary diffusion flame (Fig. 8). Very few soot particles are found at the burner exit. Comparing an adiabatic uncoupled and a non-adiabatic LES-radiation simulation, the radiation effect appeared to be rather weak in the gas phase (a difference of a few percent in the mean temperature field), but much larger in the soot volume fraction (around 35%), due to slower kinetics for the reactions responsible for the soot particle evolution.

Conclusions

The accuracy and reliability of numerical simulation, and in particular of the LES approach, have been demonstrated by considering some difficult combustion phenomena, such as ignition, combustion instabilities or pollutant emissions, in either well-controlled academic experiments or realistic, complex-geometry applications. The complementarity with experiments is clearly established and numerical simulation has now become an essential tool for research, as well as industrial design. Current and future challenges are to include even more physics, in a parallel coupled solver strategy and to extend computational domains to all elements of aeronautical gas turbines, from the compressor down to the turbine. Such objectives will be achieved with the next generation of massively parallel computers and will require important efforts on the solvers to keep them at the highest HPC standards

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Acronyms

HPC	(High Performance Computing)
DNS	(Direct Numerical Simulations)
RANS	(Reynolds Average Navier Stokes)
LES	(Large Eddy Simulations)
PDF	(Probability Density Function)
TFLES	(Thickened Flame model in the LES context)
F-TACLES	(Filtered TAbulated Chemistry for Large Eddy Simulation)
LBO	(Lean Blow-Off limits)
FAR	(Fuel-Air Ratio)
NOMANI	(Nitrogen Oxide emission model with one-dimensional MANIfold)
NOx	(Nitrogen Oxides)

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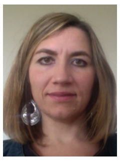

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