Modeling Challenges in Computing Aeronautical Combustion Chambers

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This article reviews the modeling challenges for performing Large Eddy Simulations of aero-nautical combustion chambers. Since the kerosene is injected in a liquid phase into the combustion chamber, the description of the atomization is of primary importance. The article first discusses the numerous numerical challenges encountered during this process, which leads to the formation of small droplets that constitute a spray. The existing numerical and modeling methods to describe a spray of kerosene droplets are then presented. The article then focuses on the description of the complex combustion kinetics. Hundreds of species and thousands of reactions have to be considered to predict ignition, flame stabilization and pollutant emissions. Due to lengthy computational times, detailed chemical schemes are too large to be directly used in CFD. This article then presents the major existing chemical reduction strategies. Significant interactions of the reactions layers with the flow vortices occur at the subgrid scale. The question of turbulent combustion modeling is therefore discussed in an LES context. Finally, the prediction of soot and NOx formation is presented. The review is illustrated by several examples representative of practical situations encountered in aeronautical combustors.

Introduction

The numerical simulation of aeronautical combustion chambers involves very complex physical phenomena. First of all, due to the high velocity of the airflow through the combustor, the reacting flow is highly turbulent. It can be numerically simulated using three levels of accuracy [1]: Reynolds Average Navier Stokes (RANS) simulations, predicting only mean flow characteristics; Large Eddy Simulations (LES), where turbulent large scales are explicitly calculated whereas the effects of smallest ones are modeled; Direct Numerical Simulations (DNS), where the full instantaneous Navier-Stokes equations are solved without any model for turbulent transfer. DNS is extremely expensive in terms of computational resources and therefore in practice is limited to simplified geometries with reduced chemical kinetics (Richardson, 2010). LES offers significant advantages when compared to RANS techniques, because unsteady large-scale motions, important for flame propagation, stabilization, flow mixing, and consequently chemical species predictions, are resolved. Also, by giving access to local and instantaneous data, it enables a better understanding and description of some complex unsteady phenomena, such as flame/turbulence interactions and pollutant formation, which are not well captured by statistical quantities. Thanks to the development of massively parallel computers, LES of practical industrial combustors, exhibiting complex geometry features, is now achievable [2].

LES of turbulent flames in an aeronautical combustor is a challenging multi-physics problem. The kerosene is first injected in a liquid phase into the combustion chamber. Due to the velocity difference between the fuel jet and the coflowing air, the liquid jet undergoes complex atomization processes, which ultimately lead to the formation of small droplets. It then constitutes a spray that feeds the flame front with evaporated fuel. The droplet size and their spatial distribution directly impact the flame position. The combustion process is also very challenging from a chemical point of view. Hundreds of species and thousands of reactions have to be considered in order to predict subtle phenomena, such as ignition or re-ignition, flame stabilization and

pollutant emissions. For computational time limitations, detailed chemical schemes are too large and chemical reductions strategies are needed to introduce reliable chemistry ingredients in LES. In practical combustion chambers the grid size is of the order of 1 mm. However, many physical phenomena occur at a smaller scale (i.e., at the so-called “sub-grid” scale) and have to be modeled. This is especially the case of chemically reactive zones, whose thickness is of the order of 0.1 mm, and the case of interactions between the flame and the turbulence. The challenges are even greater in the case of pollutant predictions because of their considerably smaller concentrations and the many pathways leading to their formation or destruction. Pollutant mole fractions amount to a few tenths to a few hundreds ppms.

The objectives here are to give an overview of the modeling challenges encountered when performing LES of aeronautical combustion chambers. The state-of-the art of liquid atomization, spray description and combustion modeling is presented. For that purpose, this article is organized as follows: Issues relative to primary atomization are first presented. The description of the liquid spray is then discussed. Chemical kinetics of kereosene/air combustion is presented in § " Kerosen chemistry modeling ", whereas § " Turbulent combustion models " summarizes the challenge of introducing detailed chemistry phenomena in turbulent flow solvers. Finally, the question of pollutant formation is developed: the prediction of soot and NOx formation are presented.

Primary atomization modeling

Atomization is a highly non-linear phenomenon that occurs when liquid fuel is injected into the combustor [3]. Primary break-up is the early phase of the atomization process when the continuous liquid core is transformed into ligaments and large droplets. The typical size of these features ranges between a few to a hundred microns. Resolving these features is presently out of reach in spray combustion simulations, which have to take into account the combustor geometry and the flame dynamics occurring at larger scales. Consequently, the impact of primary atomization on the spray formation needs to be modeled in aeronautical burner simulations.

Beyond this scale resolution issue, the simulation of primary atomization faces numerous numerical challenges: at the liquid/gas interface, the density, the pressure and the viscosity are discontinuous. Dedicated algorithms have been developed over the last decades to accurately include these jump conditions in high-fidelity 3-D unsteady simulations. The Ghost-Fluid Method proposed by Fedkiw et al [4] has been widely adopted to take into account the pressure jump at the interface without any numerical smearing. This method requires the precise location of the gas/liquid interface during the simulation. Many algorithms have been developed to track the interface and to ensure a sufficiently accurate calculation of the interface curvature and a correct mass conservation [5, 6, 7, 8]. Most of these methods have been derived within the framework of finite-differences and their application has been limited to simple geometries.

Within the framework of the European project FIRST, the feasibility of primary atomization simulation in realistic geometries has been investigated. The Accurate Conservative Level Set method [8] has been implemented in an unstructured finite-volume solver named YALES2, which is dedicated to the simulation of turbulent combustion in aeronautical burners. This methodology has been applied to several complex injectors. Two examples are shown in Figs. 1 and 2. The first configuration consists in the so-called triple disk injector [9], whose particular injector geometry creates a liquid sheet that atomizes rapidly. For this configuration, three different Large-Eddy Simulations were performed with various mesh resolutions. The finest mesh resolution, with 1.6 billion tetrahedra, enables the large-scale dynamics to be recovered as the ligament formation, but it is still not enough to capture all of the flow features from the experiment at the secondary atomization scale. The second configuration is a realistic injector provided by Turbomeca, SAFRAN Group. In this configuration, the prefilming inside an airblast swirl injector was investigated. Large-Eddy Simulations with 1.6 billion tetrahedra for 1/8th of the full geometry were conducted. Figure 2 shows the location of the interface and the velocity magnitude at the interface. While the cell count is high, the mesh resolution at the interface is not fine enough and only large-scale dynamics of the liquid sheet are captured. In this particular case, where the gas Weber number is large and the liquid sheet has large displacements, primary atomization modeling would benefit from Adaptive Mesh Refinement (AMR) methods [10] to concentrate the degrees of freedom at the interface.

Spray description

The fuel droplets generated during the atomization process are convected by the air flow and constitute a spray phase which has a great impact on the full simulation. This phase will indeed prepare the flammable mixture for the combustion process. Many questions have to be asked beforehand, such as the simulation strategy, the choices of the physical models or the boundary conditions to be used, as well as the means of validation.

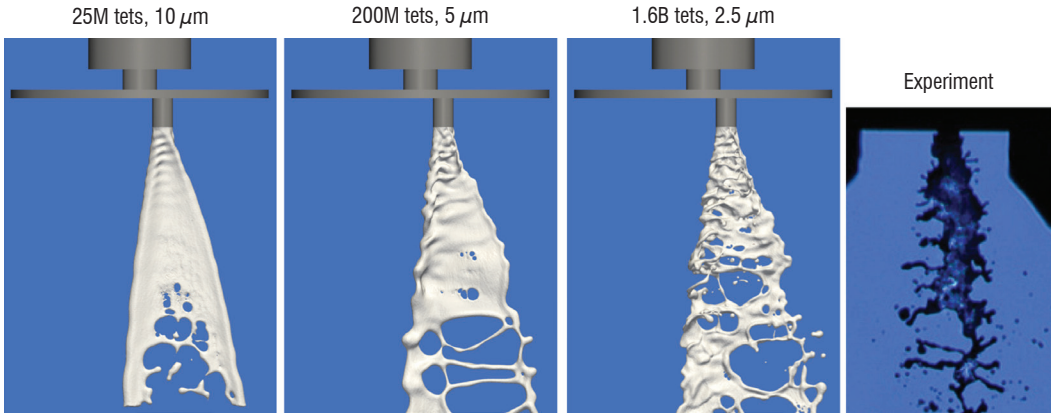


Figure 1 - Mesh refinement study of primary atomization at the exit of the triple disk injector.

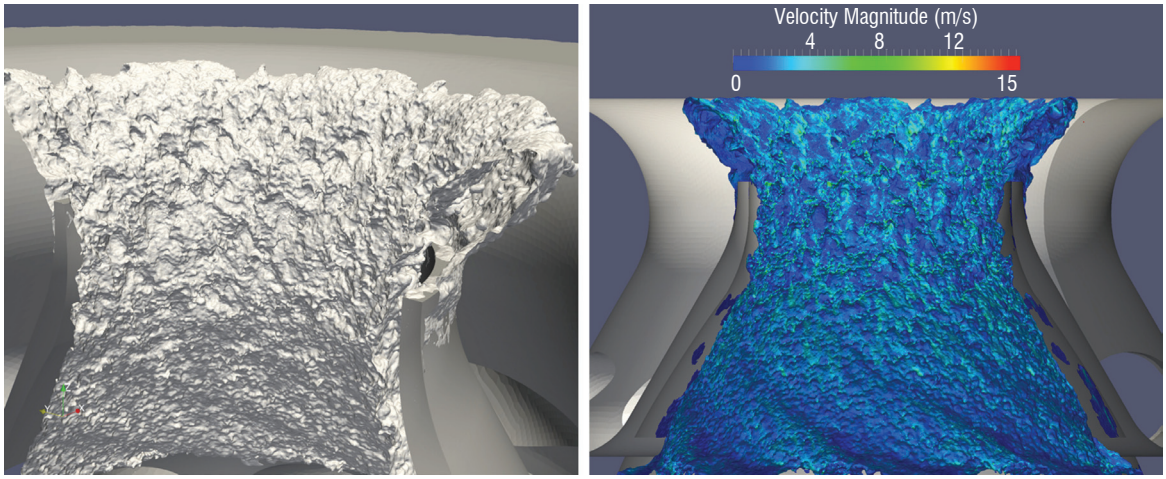


Figure 2 - Investigation of primary atomization in a realistic airblast swirl injector.

Simulation strategy

In order to describe the spray, the most commonly-used strategy is to consider a point-particle assumption, i.e., the droplet is smaller than any scale of the flow, and to use a Lagrangian Droplet Tracking method (LDT), for which individual droplets or parcels of droplets are transported by means of ODE systems on droplet state variables (position, velocity, size, etc.). To a lower extent, Eulerian methods that resolve statistical information, such as droplet concentration, are sometimes preferred for their intrinsic ability in parallel computing.

Lagrangian approaches

Lagrangian approaches are widely used because they are viewed as a reference and they also seem more intuitive than Eulerian strategies. They are based on an ODE system that solves the time evolution of the droplet state. Depending on the point of view adopted, this description may be deterministic or probabilistic. In the deterministic framework, each numerical particle corresponds to a physical droplet, and the resulting set of droplets corresponds to an individual realization of the spray. From the probabilistic point of view, the ODE system is aimed at solving a Williams-Boltzmann equation [11] on the Number Density Function (NDF). The resulting set of droplets is thus a particular discretization of a set of realizations of the spray phase, similar to Monte-Carlo simulations [12, 13], and a stochastic description must be provided for droplet evolution [14, 15].

In LES of combustors, a stochastic point of view may be required [16], in which the parcels will represent sets of physical droplets. At this point, the choice of the best statistical representation in terms of parcels [13] is not straightforward and not necessarily unique, adding a degree of freedom to Lagrangian computations. Paulhiac [17] highlights this issue and proposes strategies for the statistical distribution of parcels. However, the most effective solutions in the literature are case-dependent and a statistical convergence verification is still required for Lagrangian simulations. Aside from that, efforts on the parallel efficiency of Lagrangian simulations are certainly of interest, for example using task-oriented paradigms or dual-constraint decomposition [18].

With regard to the numerical resolution, one important source of error is the projection strategy used to exchange droplet source terms with the gas phase. Actually, the classical point-particle approach cannot ensure mesh convergence. Strategies have been proposed in the literature [19, 20] to overcome this, using for instance Gaussian projection with a mesh-independent width. This kind of approach needs to be adapted to unstructured grid simulation, like in [17], and a more careful analysis and justification of the projection kernel, linked to the resolved scales for instance, needs to be carried out.

Finally, an interesting issue is the modeling of sub-grid scale effects on two-way coupling between carrier phase and disperse phase. In the literature, models have been devised to take into account the impact of sub-grid scales on the droplet motion [21, 16, 22], and have been applied to combustors simulations [23, 24]. However, no model has yet been developed to account for the effect of the disperse phase on the carrier phase sub-grid scale, either in the dynamics or in terms of temperature and composition. Such a development may be of great interest due to its link to the mixture formation and, consequently, the combustion process.

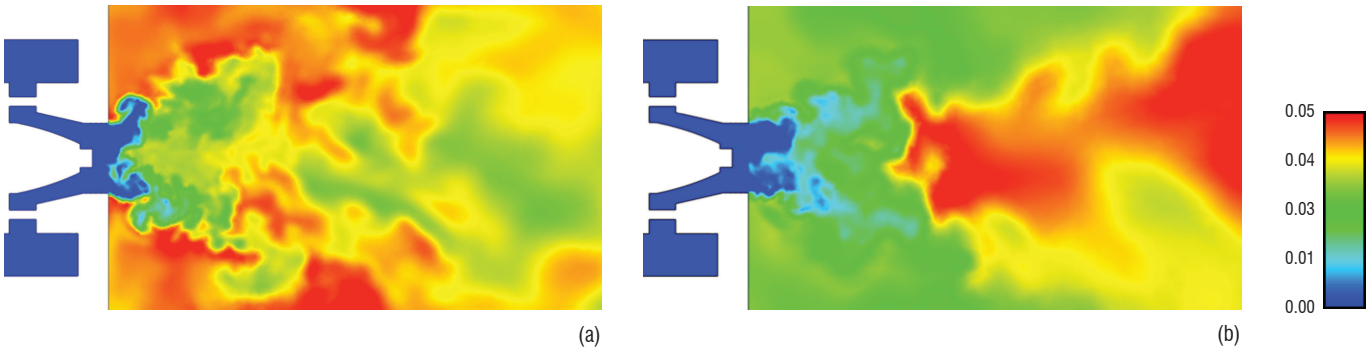


Figure 3 - Simulation of the MERCATO test rig of ONERA [34]. Vapor fuel mass fraction obtained with (a) mono disperse and (b) multifluid models for non-reactive conditions.

Eulerian Moment methods

Compared to Lagrangian methods, Eulerian approaches have the advantage of solving a fluid description similar to the gas phase, which enables the use of the same type of parallelism algorithm. Moreover, statistical convergence is intrinsically achieved, sine Eulerian methods directly solve the moments of the NDF. However, they come with two drawbacks compared to Lagrangian methods. First, moment methods need closures for the moment system, since for any moment set higher order moments are required to close the fluxes. The closure must be dictated by the physics of the problem and will induce a modeling error that does not exist for Lagrangian methods. Second, moment methods lead to a system of partial differential equations for which specific numerical methods have to be used in order to reduce numerical dissipation. For the simulation of aeronautical combustors, the two most important issues are the description of the size polydispersion of the droplets and the robust and accurate numerical resolution of the moment system on unstructured grids and complex geometries.

Concerning the size polydispersion, injection strategies can lead to polydisperse sprays with droplet sizes ranging from one micron to 200μm, and this polydispersion persists inside the combustion chamber. Simulations [25, 26] have exhibited the impact of size polydispersion on the spray and, for instance, experiments from [27] have identified the polydispersion as a potential origin for flame stabilization or flame bifurcation because of size-conditioned dynamics. In the literature, many polydisperse Eulerian strategies are available, ranging from Multifluid methods that discretize the size space into sections, to high order moment methods, see [28, 29, 30, 31, 32] and references therein. However, even though high order moment methods have been used for automotive engines [33], the only method that has been used to describe the cold flow of an aeronautical configuration is the first order Multifluid method [26], see Fig. 3, which is still expensive since 10 sections are required. The second order Multifluid method of Laurent et al [32.1, 32.2, 32.3] used for solid propulsion in the CEDRE code is for now the most attractive strategy, which reduces the required number of sections.

Concerning the numerical resolution of the moment equations, several works have evidenced the difficulty to accurately and robustly solve moment equations in complex configurations and unstructured grids using conventional methods (see [35] and references therein). In fact, due to the droplet phase inhomogeneity induced by the injection and the turbulence, the disperse phase exhibits strong gradients and vacuum zones. This requires the use of stabilization techniques, such as artificial viscosity or flux limiters, which still need an iterative process to adjust numerical parameters in order to obtain the best solution. A major challenge is thus to design numerics that are intrinsically stable and robust. In the literature, the only works that deal with the numerics of Eulerian methods on unstructured grids have been performed in the AVBP code of CERFACS and the CEDRE code of ONERA. The former is based on a Taylor-Galerkin scheme [36] initially developed for the gas phase. For Eulerian simulations, specific attention has been given to artificial diffusion operators, in order to stabilize the simulations [37, 38, 39]. The latter uses a realizable multislope MUSCL method [40] adapted to two-phase flows, which is limited to second order accuracy. In order to achieve sufficient accuracy while ensuring robustness, a method of great potential is the Discontinuous Galerkin (DG) approach. For example, in [41], it has been shown that it is possible to design DG schemes [42] for moment equations that satisfy all stability requirements as well as strongly increasing accuracy compared to the MUSCL strategy, even at second order.

Apart from these two issues, velocity and temperature polydispersions, especially in the context of LES, will have to be properly modeled. For these two issues, two types of strategy exist. The Algebraic-Closure-Based Moment Methods (ACBMM) [43, 44] model the unclosed terms using information on moments and have already been used to simulate complex configurations using the AVBP code [45, 46, 26]. The Kinetic-Based Moment Methods [47] use assumptions regarding the underlying kinetic distribution. A comparison has been made in [48], showing that both methods have a close level of accuracy, with ACBMM having an advantage in terms of number of equations (5 against 10 in 3D) and KBMM having an advantage in terms of numerics (hyperbolic structure of the equations [49]). The extension of such models to two-way coupling has yet to be proposed, since it is essential for combustion problems, and should be inspired by previous work in the RANS context [50, 51].

Physical models

In order to describe the spray evolution, the physical processes that affect the spray must be defined. The spray regime encountered in combustors restricts the most important processes to the drag force and the heat and mass transfers, since these are the most likely to drive the spray trajectory, as well as its exchanges with the gas phase. The most widely used model to express the drag force is the Schiller-Naumann correlation [52], which acts as a Reynolds-based correction of the classical Stokes law [53] and has been shown to be valid in the diluted regime. At this point, the most prominent question for drag force is whether or not to evaluate one of its parameters: the unperturbed gas velocity. In [54], the authors point out this issue by demonstrating that, even in the point-particle limit, the model should not directly take the gas velocity at the droplet location as an unperturbed velocity. Such a modification should be more deeply tested and evaluated in real applications, in order to see its impact. Concerning heat and mass transfers, a wide range of models can be found in the literature, with different sets of assumptions and different validation cases. A comprehensive review is available in [55]. Many recent models have been focused on the evaluation of the gas phase properties at the droplet surface, by considering for instance complex transport in the case of reduced chemistry [56] or corrected Stefan fluxes [57]. Shashank et al [58] have also investigated the sensitivity of models to the 2/3-1/3 approximation [59] for gas phase reference quantities, and have shown the great impact of this choice. In the end, the most difficult issue is the validation of the evaporation model with regard to reference experiments. First, designing an experiment to evaluate vaporization is not straightforward. For instance, Chauveau et al [60] have demonstrated the impact of the support fiber to be non-negligible. Second, most droplet evaporation experiments are performed on pure hydrocarbons, and more data are required for kerosene under various conditions. Third, the impact of droplet motion as well as droplet combustion on the vaporization correlations must be properly validated for kerosene under realistic conditions. For example, a model for taking into account isolated droplet combustion has been proposed in [17].

Physical processes besides evaporation and drag force should also be taken into account. For instance, droplet secondary break-up modeling can have an impact on simulations [61] and would need further

investigations regarding the numerous available break-up models, see for instance [62] and references therein, for the sensitivity to the chosen model. Models for droplet/wall interactions, as well as film formation and break-up, would also be of interest, since many injection devices could lead to the impact of the jet in the swirler region or at the combustion chamber walls. Such a physics is not straightforward to handle, since it would require the film formation from droplet impacts to be modeled, as well as the film breakup into droplets. In the work of Chaussonnet et al [63, 64], the authors proposed a first model to account for such a transition by describing the film formation from Lagrangian droplets and modeling the droplet generation from the film break-up.

Injection modeling

Although it is not possible at this time to simulate the primary atomization process from the injection location to the combustion chamber, two-phase combustion chambers have been simulated over the past decade by using boundary conditions for the disperse phase: instead of injecting a coherent liquid jet, boundary conditions are moved downstream into the disperse phase region, and a distribution of droplets is injected [21, 65, 66, 24]. In order to choose the appropriate profiles at the boundary condition, models have been devised based on phenomenological models and appropriate volume balances. However, these models still rely on experimental data to adjust parameters such as droplet diameters, in general taken at the closest measurement location. Such a solution is helpful to run computations, but is not a long-term solution since experiments will always be needed to adjust the injection model. In order to avoid these constraints, the most evident solution is the use of high-fidelity injection simulations that accurately reproduce all of the features of the primary atomization process, in order to provide more insightful descriptions of the injection system, for instance by giving the droplet size distribution from the injection exit. In addition to the development of boundary conditions, methods are also under development to ensure the transition between the separated and disperse phases, and will be a building block for future complete simulations, see [67, 68, 69.1, 69.2, 69.3, 69.4] for instance.

Validation

Finally, an important point concerning disperse phase simulations relates to the validation strategy. Actually, due to the complexity of the physics and the difficulties in accessing information in a reactive configuration, particular attention must be paid to this specific issue. Actually, two ANR projects were initiated this year, which will give a specific focus on this issue. First, the project named NEXTFLAME (EM2C/CERFACS) will investigate two-phase combustion in a counterflow burner, for which a detailed characterization of inflow conditions and spray flame characteristics will be available. Second, the TIMBER project (EM2C/CERFACS/CORIA/SAFRAN) will investigate two-phase ignition in annular chambers, and for this purpose will use simple benchmark cases. Both projects will give the community reference test cases that will possibly be used for in-depth validation of simulation strategies.

Kerosene chemistry modeling

From a chemical kinetic point of view, the combustion of aviation fuels is a challenging problem. Jet fuels, such as Jet A-1 and JP-8, are complex mixtures of over one thousand hydrocarbons containing from 8 to 16 atoms of carbon. Moreover, the chemical composition of a given jet fuel can vary and different fuels are used world-wide with compositions that differ significantly from one location to another. Finally, jet fuels also contain additives (such as antioxidants, corrosion inhibitors or metal deactivators), which are determined by the specific use of the fuel. Both the physical properties of the jet fuel and its global reactivity, as well as its propensity to produce different pollutants such as soot, depend on this composition. Due to the complexity of these mixtures, the detailed composition cannot be used as an input for combustion modeling purposes. Until the last decade, aviation fuel combustion was modeled using a single component. After reduction, the chemical kinetic mechanism fits CFD requirements well, especially in terms of number of species. With the continuing increase of computer power and the interest in alternative aviation fuels whose chemical composition again differs from that of conventional jet fuels, new strategies were developed to better predict heat release and pollutant formation during the combustion in gas turbine engines. These strategies rely on the idea that all of the individual hydrocarbons present in a jet fuel (conventional or alternative) can be classified into four different families: n- and iso-paraffins, naphthenes and aromatics, with relative abundances depending on the fuel. All of these families have specific chemical reactions and different reactivities. A so-called surrogate can be formulated as a mixture of well-chosen hydrocarbons representative of their own family. A first approach was developed by Guéret et al [70] with a mixture of three hydrocarbons (79% n-undecane, 10% n-propylcyclohexane, 11% 1,2,4-trimethylbenzene) to model the oxidation of a Jet A-1 in a jet-stirred flow reactor at atmospheric pressure. It was found that the identified reaction products formed during the oxidation of the ternary mixture and the kerosene were very similar in terms of concentration. Furthermore, a quasi- global chemical kinetic reaction mechanism was developed to reproduce the experimental data. The authors concluded that a kinetic model involving an equivalent mixture of a small number of pure hydrocarbons can represent the oxidation of kerosene.

Then, Dagaut et al [71] formulated four chemical surrogate model fuels of increasing complexity from pure n-decane (100%mol.), n-decane/n-propylbenzene (74%/26%mol.), n-decane/n-propylcyclohexane (74%/26%mol.) and n-decane/n-propylbenzene/n-propylcyclohexane (74%/15%/11%mol.). The oxidation of these four mixtures was studied in a jet-stirred reactor at atmospheric pressure, over a temperature range from 900 to 1300 K and variable equivalence ratios, and compared to the oxidation of Jet A-1 obtained under the same conditions. It was found that the 3-component fuel model was the most appropriate to simulate the jet stirred reactor experiments, as well as a fuel-rich premixed kerosene-oxygen-nitrogen flame. In 2006, Dagaut and Cathonnet [72] published a review of kerosene combustion in which they reported recent advances on the formulation of kerosene surrogate fuels, as well as experimental kinetic studies on kerosene and surrogate ignition, oxidation and combustion and the latest kinetic modeling efforts. The relevance of the approach using chemical families was demonstrated through numerous simulations of Jet A-1 and JP-8 surrogate combustion, but the authors highlighted the lack of experimental data under flame conditions. A similar initial idea by Colket et al [73] was to design a simplified surrogate composed of n-decane (50%vol.), n-butylcyclohexane (25%vol.) and n-butylbenzene (25%vol.) to better match the hydrogen/carbon ratio (1.91 for JP-8) and set the aromatic content at the limit of the aviation fuel regulations. Ignition temperature, extinction strain rates and CO mole fractions were

measured and this group concluded that this surrogate was more reactive and more difficult to extinguish than typical jet fuels. Finally, a roadmap was proposed for the development of jet fuel surrogates. The targets identified by Colket et al [73] were pushed further by Dooley et al[74]. They decided to focus the design of comprehensive surrogates not only on the H/C ratio but also on the derived cetane number (DCN), the threshold sooting index (TSI) and the molecular mass. They started with fourteen different mixtures of n-decane, iso-octane and toluene. DCNs were measured using an ignition quality tester and TSIs were determined from a linear relationship taking into account the TSI of pure components and mixture fractions. Finally, their surrogate was composed of n-decane (42.67%mol.), iso-octane (33.02%mol.), and toluene (24.31%mol.). They measured mole fraction profiles in a flow reactor and ignition delays in a shock tube and a rapid compression machine at high pressures, and strained extinction limit of diffusion flames for both their surrogate and a Jet A fuel. It was found that such a surrogate was able to closely emulate the global combustion parameters of the Jet A fuel chosen in the study (POSF 4658), as well as the chemical kinetic related behavior, even though they admitted that the present surrogate did not exactly match all of their goals. More recent works have addressed the combustion of alternative jet fuels, for instance through Alfa-Bird (Alternative Fuels and Biofuels for Aircraft Development), a European Union funded research project testing biofuels and alternative fuels as a means of ensuring the long-term viability of the international air transportation industry. Mzé-Ahmed et al [75] studied the oxidation of a coal-to-liquid Fischer-Tropsch synthetic jet fuel and compared it to a quaternary mixture made of n-decane (47.2%mol.), iso-octane (15.5%mol.), n-propylcyclohexane (42.2%mol.) and n-propylbenzene (12.2%mol.). They concluded that the surrogate represented the oxidation of the synthetic jet fuel reasonably well, but that it required more realistic alkanes and naphthenes to be involved. This conclusion was emphasized by Dagaut et al [76] studying the oxidation of gas-to-liquid Fischer-Tropsch synthetic jet fuel. As compared to the GtL, the surrogate (65.2%mol. n-decane, 37.5%mol. iso-octane and 10.3%mol. n-propylcyclohexane) was shown to have a similar reactivity but some species (iso-butene) were largely over-estimated, indicating that iso-octane might not be a good representative compound of the iso-alkane family. In the most recent works [77], a fraction of iso-octane has been replaced by a mixture of 2-methylheptane and 3-methylheptane, in order to better match the combustion behavior of the iso-alkane family. Also, decalin and tetralin have been introduced into the composition of the surrogate in addition to n-propylcyclohexane and n-propylbenzene, in order to achieve a more realistic representation of the naphthene and aromatic families. This flexible detailed kinetic mechanism was able to successfully reproduce the oxidation of a GtL and a CtL under high pressure and from fuel-lean to fuel-rich conditions. The interest of such a flex-fuel kinetic mechanism is that it can be reduced on purpose (for one typical fuel, under few thermodynamic conditions) to match CFD requirements.

Turbulent combustion models

Chemistry reduction

An accurate prediction of the temperature evolution and the species formation across a flame requires a reliable description of chemical mechanisms. Detailed schemes correspond to an exhaustive list of all possible elementary reactions between a given fuel and an oxidizer. However, as explained in Section 4, detailed kerosene/air reaction schemes involve hundreds of species and thousands of elementary reactions. Despite the continuous increase in computational power, detailed chemistry flame computations remain prohibitive for practical aeronautical combustors. In practice, detailed chemistry computations are mainly applied to 1-D laminar kerosene-air flames [78] and 3-D DNS of turbulent flame, but limited to small domain size and Reynolds number, and to light hydrocarbons [79].

Identification of a skeletal mechanism

For this purpose, methods have been developed to reduce the chemistry. The first reduction step is the identification of a skeletal mechanism where, for a given range of parameters, unimportant reactions and species are suppressed. Methods for the systematic reduction of mechanisms to a skeletal level have been proposed in [80, 81, 82, 83]. The resulting skeletal mechanisms are still in general too large to be included in 3-D reactive flow simulations. A second reduction step is therefore needed for practical simulations.

Popular procedures to systematically reduce mechanism are the Quasi Steady-State approximation (QSSA) and/or the Partial Equilibrium approximation (PEA). QSSA assumes that the rates of production and destruction of a selection of species are much greater than their net rate of formation. This yields algebraic relations for production rates of these species among the elementary rates. The PEA assumes that the rates of some reactions are so high that partial equilibrium is established, also giving rise to algebraic relations between the elementary reaction rates. An extensive description of these methods, together with the mathematical framework and illustrations with practical examples, is given in the review article [84].

One of the first attempts to reduce detailed schemes within the context of kerosene chemistry was performed by Luche et al [85]. From a detailed mechanism comprising 225 species and 3493 irreversible reactions proposed previously, the authors first obtained a skeletal mechanism including 134 species and 2132 reactions by using atomic flux analysis. This skeletal mechanism was further reduced to 1220 reactions by removing redundant reactions with the principal component analysis method. A last step was applied using the quasi-steady-state approximation for species with a short lifetime, and two reduced schemes including 33 and 40 species were finally obtained. These reduced mechanisms offered a good compromise between predictive qualities and computation time. Another example of a reduced mechanism is given in [86]. The skeletal JetSurF 1.0-l1 mechanism [87][1], including 123 species and 977 reactions has been systematically reduced using a directed relation graph (DRG), DRG-aided sensitivity analysis, and linearized quasi steady state (QSS) approximations, leading to an analytical 24-species mechanism for n-dodecane.

Empirically-reduced mechanisms

An alternative to describe combustion chemistry is the use of empirically reduced mechanisms. These ad hoc models composed of one to four steps are built to reproduce global flame properties, such as the laminar flame speed, the burnt gas composition or the auto-ignition

[1]JetSurF 1.0-l1 is already a simplified version of JetSurf 1.0 [88]

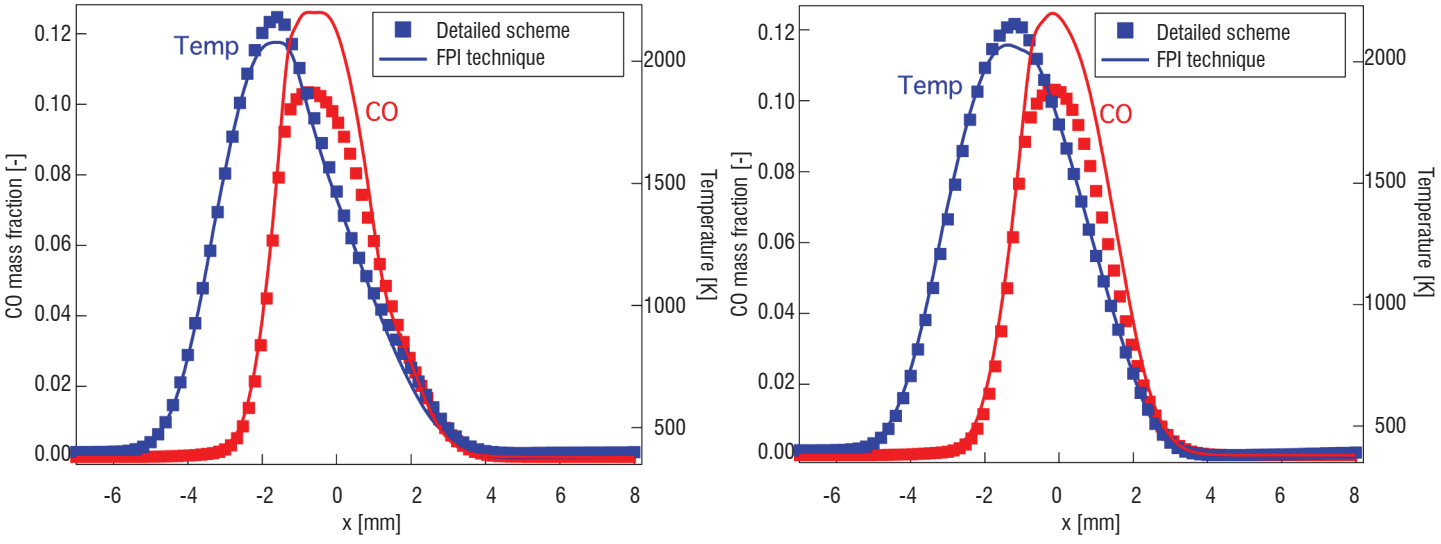
times. Reaction rates are determined by tuning, guessing and trial and error. Pioneering work is due to Westbrook and Dryer [89], who proposed one and two-step global reactions with Arrhenius kinetics by tuning the pre-exponential factor, the activation energy and the reaction order. More recently, the applicability of one-step irreversible Arrhenius kinetics with unity reaction order to the description of partially-premixed methane-air combustion has been investigated in [90]. For more complex hydrocarbons, a simple technique has been proposed [91, 92] to derive one-step and two-step schemes for kerosene-air flames. In order to fit the laminar burning velocity over a wide range of operating conditions, the pre-exponential constants of the two reactions are tabulated as a function of the local equivalence ratio. The fuel and oxidizer exponents are adjusted to reproduce the dependence of premixed laminar burning velocity on mean pressure. However, the optimization of these mechanisms remains limited by the thermochemical properties of the species involved, which remain unchanged. A solution to overcome this issue is to develop virtual schemes involving virtual species and reactions [93]. The use of virtual species, whose thermodynamic properties are optimized, improves the domain of validity of global step mechanisms.

Tabulated chemistry methods

An alternative to address fluid/chemistry interactions at a reduced computational cost consists in tabulating the chemistry. A chemical look-up table is generated prior to a CFD simulation, in which main thermo-chemical ingredients are stored as a function of a reduced set of variables. Some techniques to construct the chemical look-up table, such as the Intrinsic Low Dimensional Manifold (ILDM) developed by Maas and Pope [94], are based on a mathematical reduction of the chemical system dynamics. However, a large number of coordinates, around four or five, are required when hydrocarbons fuels are considered. Alternatives to ILDM that require less dimensions are Flame Prolongation of ILDM (FPI) [95, 96] or Flamelet Generated Manifold (FGM) [97]. Both techniques assume that the chemical flame structure can be described by a reduced phase subspace from elementary combustion configurations. For instance, the chemical subspace covered by partially-premixed flames can be approximated from a collection of 1-D laminar flames [98].

The suitability of tabulated chemistry for kerosene combustion has been recently investigated by simulating 1-D laminar spray counterflow flames [99]. Figure 4 shows a comparison between detailed and tabulated chemistry simulations. Both methodologies use the same skeletal mechanism developed by Luche [85], so only assumptions relative to chemistry tabulation are challenged. The temperature profile is well reproduced by the tabulated chemistry method, but small discrepancies are observed in the CO prediction. These errors are due to the fact that a single flame archetype (premixed flamelets) is used to build the chemical look-up table, whereas the structure of the spray counterflow flame is more complex. This assumption, valid to capture the temperature, is too crude to capture complex chemical phenomena, such as the pollutant formation.

This result illustrates the limitation of tabulated chemistry methods, which assume that a turbulent flame is composed of a set of laminar flame elements. The identification of the combustion elements representative of the overall turbulent chemical flame structure is not always obvious. The use of a single flamelet archetype is efficient to capture the chemical structure of well-identified flames (such as purely premixed flames or diffusion flames), but introduces bias in the prediction of the chemical structure of more complex situations such as stratified flames [98]. In order to capture the complex flame structures that develop in the reactive flow, more coordinates have to be added to the look-up table. In order to track multiple flamelet regimes within a single look-up table, Bykov and Maas [100] and Nguyen et al [101] proposed to solve the projection of the full set of species balance equations in a restricted subset of the composition space. Another solution, suggested recently by Franzelli et al [78], is to combine partially-premixed flamelets to generate a chemical look-up table.



(a) 40 μm droplet diameter

(b) 100 μm droplet diameter

Figure 4 - Chemical flame structure of a 1-D laminar spray counterflow flame using a detailed chemistry (solid) and a FPI tabulated chemistry approach (symbols).

LES of turbulent combustion

Two major issues must be overcome to perform LES of turbulent combustion:

- The flame thickness is typically thinner than the grid size. Indeed, the flame reactive layer is usually about 10-100 micrometer wide, while the filter size remains above 1 millimeter [102].

- Part of the flame wrinkling induced by the turbulence is not resolved by the LES. Therefore dedicated models for flame/turbulence interactions are needed [1].

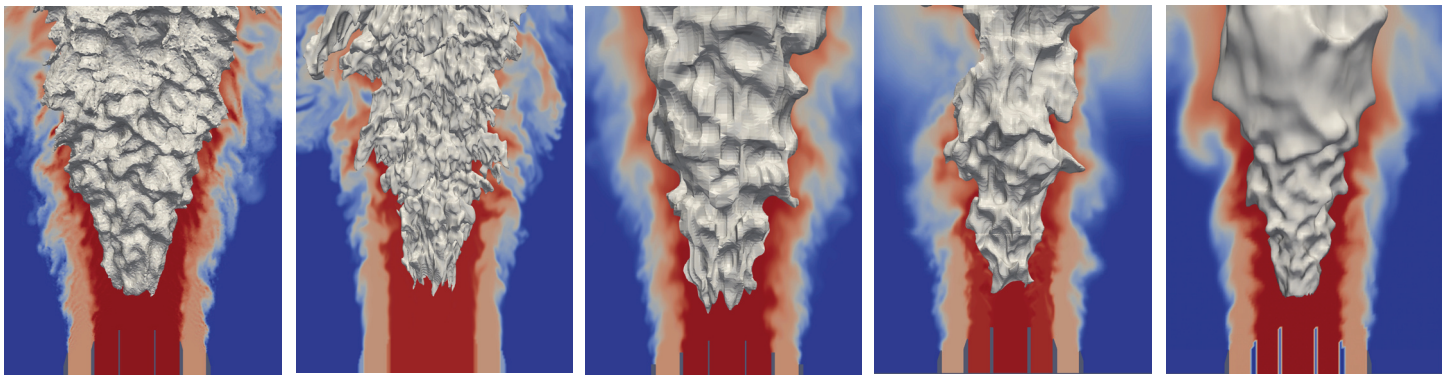
Regarding the first point, an efficient solution to solve flame propagation on a coarse grid is to artificially thicken the flame front by modifying the diffusion coefficient and the Arrhenius pre-exponential constant [103, 104]. This methodology, which is straightforward to implement in a LES solver, has been successfully applied on gas turbine combustion chambers, both within the context of global-step chemistry [105] and that of tabulated chemistry [106]. Another solution is to introduce a filter larger than the mesh size, in order to resolve the filtered flame structure. This method has been followed by Boger et al [107] and Duwig et al [108] with a single-step description of the chemistry. This strategy has been followed within the context of tabulated chemistry with the development of the F-TACLES (Filtered TAbulated Chemistry for Large Eddy Simulation) model, which was first formulated for premixed [109], then stratified adiabatic [110] and non-adiabatic combustion [?]. This modeling strategy has been applied by [111] to understand the formation of the hot regions observed at the wall surface of a helicopter combustion chamber. Another approach is to solve a scalar field, where an iso-surface is defined to represent the instantaneous flame front position. This method called "G-equation" was first applied to LES in [112]. The mathematical formalism of the G-equation has been updated for LES in the corrugated flamelet regime [113] and in the thin reaction zones regime [114]. The G-equation model has been coupled to tabulated chemistry in [115].

The second issue concerns the sub-grid flame/turbulence interaction modeling. Indeed, the turbulence of the flow generates vortices (or eddies), which wrinkle the flame front over a wide range of length scale. In practical LES computation grids, a significant part of the flame wrinkling occurs at the sub-grid scale and requires modeling [1]. Significant progress has been recently achieved with the development of dynamic sub-grid scale models [116], which have been successfully coupled with the flame filtering concept [117, 118]. They demonstrate that this combination is very efficient to predict the flame stabilization process and the temperature distribution in the combustion chamber.

Some above mentioned methods have been recently challenged in a collaborative study in which five research institutions have been involved to simulate a turbulent stratified flame (TSF) measured at the Technische Universitt Darmstadt (TUD) [119]. The groups involved in the simulations are TUD, the Institute for Combustion Technology (ITV, Aachen), Lund University (LUND), the EM2C laboratory at Ecole Centrale Paris (EM2C) and Duisburg-Essen University (UDE). All groups performed Large Eddy Simulations using Low Mach Number solvers. EM2C employed the Filtered Tabulated Chemistry for LES (F-TACLES) model [109], extended to capture the propagation of non-adiabatic flames [120]. TUD applied a premixed flamelet tabulation with local flame thickening [119]. ITV used a flamelet progress variable approach also based on premixed flamelet tabulation, but coupled with a level set approach [115]. LUND described the combustion chemistry through a 4-step mechanism combined with Implicit LES [121]. UDE used an artificially-thickened flamelet generated manifolds technique on many low cost cells.

These computational strategies differ by many aspects of numerics, turbulent combustion models and meshing. However, all modeling strategies were designed to produce the correct laminar flame speed under non-adiabatic conditions. Most simulations agree on the mean flame brush position, but it is clear that sub-grid turbulence must be considered to achieve the correct turbulent flame speed. Instantaneous snapshots of the flame, shown in Fig.5, illustrate the ability of the methods to capture the flame lift-off height. Discrepancies in the flame wrinkling resolution are caused by the different grids and numerical methods, as well as by the various LES combustion models used.

An alternative, adapted to the simulation of high Reynolds moderate Damkohler number turbulent flames [122, 123], is to use LES-EPaSR (extended Partially Stirred Reactor) and RANS-EPaSR models, which incorporate the influence of finite rate kinetics. It is assumed (similarly to the EDC model of Magnussen) that chemical reactions take place only in the fine vortex structures, characterized by high intensity



(a) EM2C (b) UDE (c) ITV (d) LUND (e) TUD

Figure 5 - Instantaneous snapshots from non-adiabatic simulations of the TSFA flame: 3-D views of 1850 K temperature iso-surface conditioned on the flame surface. 2-D field showing the mixture fraction iso-contours.

velocity gradients, molecular mixing and dissipation. Using the similarities with the mathematical treatment of multiphase flows, equations are derived for the fine-structure composition and volume fraction, which are solved together with the LES or RANS equations for the resolved scales. If convection and unsteady effects can be neglected, the EPaSR model is reduced to the PaSR model. The EPaSR model was validated against experimental data, e.g., lean premixed bluff-body stabilized flame, supersonic combustors and many other cases [122] [123] [124] [125].

Pollutant formation

Soot

Soot particles are solid fractal aggregates of small size caused by an incomplete combustion of hydrocarbons. Not only do they have a negative impact on health and the environment, but they can also cause a significant loss of efficiency of aeronautical combustors due to soot radiation, deposits and wall deterioration. Soot production is the result of complex processes of both formation and destruction, including the generation of first nuclei from gaseous precursors (the polycyclic aromatic hydrocarbons - PAHs), gas-solid and solid-solid collisional processes (condensation and coagulation, respectively) and chemical reactions at the soot particle surface (surface growth and oxidation) [126]. Therefore, soot production depends on the fuel used, the mixture quality, the operating point and the combustion mode. It is generally characterized by the soot volume fraction and the particle number density, giving access to a mean soot particle diameter. However, the particle size distribution (PSD) provides a better description of soot emission, although it requires more sophisticated experimental diagnostics and detailed numerical models to be analyzed and/or predicted.

Today, using numerical simulations to predict soot production in aeronautical combustors is extremely challenging for different reasons:

- Complexity of the physical process: due to the complex nature of soot production, detailed models are required to describe both the gaseous and the solid phases [127, 128, 129]. Such detailed models are prohibitive in real systems and simplified descriptions are required. However, the simplification procedure is not straightforward and may lead to strong inaccuracies on soot prediction.

- Multi-physics coupling: soot production strongly depends on the flame structure, the concentration of soot precursors and radicals, as well as the temperature. Acceptable discrepancies with regard to gaseous predictions lead to large errors on soot production. As an example, overestimating the precursor concentration by twice the amount leads to an overestimation by one order of magnitude of the soot volume fraction [130]. Therefore, high fidelity models are necessary for the gas phase chemistry and flame-turbulence interactions. Moreover, the presence of soot in the flame is a major source of radiative heat transfer. The non-linear coupling between soot particles and radiation must be correctly reproduced to accurately predict soot production [131], requiring the use of multi-physics coupling strategies.

- Lack of experimental databases for soot production in real combustors: this is mainly due to the difficulties in achieving measurements for both the gaseous and solid phases [132]. In academic turbulent flame configurations, Laser Induced Incandescence (LII) is the main technique used to non-intrusively measure the time-resolved soot particle volume fraction [133, 134, 135]. Combined diagnostics are increasingly being used to investigate the relation between soot, on the one hand, and flow dynamics, soot precursors and the front flame on the other hand [136, 137, 138]. High speed measurements also enable the soot-turbulence interaction [138, 139] to be characterized. Applying such diagnostics to realistic geometries is still very complex. It has recently been done for the first time at DLR by Geigle et al [140, 141, 142] in a swirled turbulent ethylene-air non-premixed flame at moderate pressure (3 and 5 atm). By combining LII, soot luminosity, OH fluorescence (PLIF) and luminosity, Particle Image Velocimetry (PIV) and Coherent Anti-Stokes Raman Spectroscopy (CARS), the DLR database offers a detailed characterization of the flow, the flame structure and the soot production for soot modeling validation.

Despite these difficulties, soot production in an aeronautical burner has been investigated using both Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES).

First attempts to predict soot production in real gas turbine combustors were based on RANS [143, 144, 145, 146, 147, 148], whose accuracy was quite limited. This approach is however not suitable for soot formation prediction because this complex phenomenon is controlled by local and history-dependent processes that cannot be modeled by RANS [135].

Since LES captures the temporal and spatial evolution of the local flow structures, it is a valid alternative. The first LES of soot production in turbulent laboratory-scale flames have proven the potential of this approach at a reasonable computational cost [149, 150, 151]. Aimed at real combustors, LES was recently performed in the DLR aero-engine model combustor [130, 152] (Fig. 6), using a semi-empirical two-equation soot model [153]. As for the gas ethylene-air chemistry, both a fully tabulated method and a hybrid method (two-step reduced

Figure 6 - LES of the DLR swirled turbulent flame [130].
Isocontour of temperature colored by the axial velocity (red-to-yellow) and soot ligaments colored by their number density (black-to-white).

chemistry for the flame-tabulated chemistry for the soot precursors) [154] were evaluated. Comparisons with experiments showed correct agreement in terms of soot position, but large differences in terms of soot levels in the combustion chamber. The sensitivity of the soot volume fraction to the gas chemical description was analyzed [130, 152].

As for real aeronautical burners, the first LES computation was proposed by Mueller and Pitsch [155], based on a tabulated chemical description for the gaseous phase and on a method of moments for the solid phase characterization. Radiation was accounted for via a simple optically thin approach. Lecocq et al [154] proposed the first LES of soot production in a real helicopter combustion chamber coupled with a thermal radiation solver. This simulation, based on an hybrid model for the gas and on a semi-empirical two-equation soot description, enabled the effect of soot radiation on the prediction of the soot volume fraction and the soot number density to be studied. Due to the unavailability of experimental results, it is not possible to make any statement regarding the accuracy of these calculations.

Despite the feasibility of LES for soot production modeling, the models both for the gas and the solid phases must be largely improved and their validation must be extended to measurements in real aero-engines. Some of the most relevant improvement pathways are suggested in the following. The list is however not exhaustive, due to the multi-physics complexity of the problem:

- Gaseous phase description and its coupling with soot: a correct description of the gaseous phase, i.e., temperature, PAH and intermediate species such as OH, is essential to predict the chemical soot production processes. Detailed chemistries are not affordable in LES of complex burners, requiring reduction procedures to account for large PAHs, strain rate effects on soot precursors and soot feedback on the gaseous phase. Tabulated methods and hybrid techniques are promising ways to be explored [154, 156, 157, 158, 159].

- Descriptions of soot PSD: with regard to spray flames, both Eulerian approaches (sectional models, method of moments and hybrid methods) and Lagrangian models should be preferred to semi-empirical models to describe soot particle population (see § " Spray description "). Among them, the method of moments, which offers a good comprise between computational cost and accuracy, is the only PSD model that has already been applied in a LES of a aero-engine combustor. This strategy has been widely developed for soot prediction [160, 161], enabling a possible extension to a bi-variate volume-surface description that can account for the fractal nature of soot. The capability of the other techniques to reproduce PSD evolution in real applications is still to be shown.

- Soot-turbulence interaction: soot production in turbulent flames is characterized by the presence of small pockets or ligaments [138, 162]. Such structures cannot be resolved on the grid accessible today in numerical simulations of realistic applications. Suitable sub-grid models accounting for turbulence effects on soot [163] are required in order to correctly reproduce the spatial evolution of soot, as well as its intermittency.

- Accounting for detailed soot radiative properties: soot radiation may contribute greatly to the total heat flux of a combustor chamber, consequently affecting the flow temperature field and soot production causing a non-linear feedback. A detailed description of soot radiative properties, based for example on particle morphology or composition [164], should be accounted for and coupled with the flow solver.

- Extension to realistic conditions: most of the modeling developments, as well as the experimental measurements, are focused on simple fuels, such as ethylene or methane, or are for simpler operating conditions (low pressure for example). The DLR experimental database, for example, concerns ethylene flames up to 5 atm. Research activities under realistic conditions for a kerosene surrogate is an active on-going topic, which should provide a better insight of soot production and lead to more accurate models.

Due to the complex nature of soot, new models must be expressly developed to reproduce the solid phase characteristics. Such developments are expected to notably improve the numerical prediction of soot production in real aero-combustors.

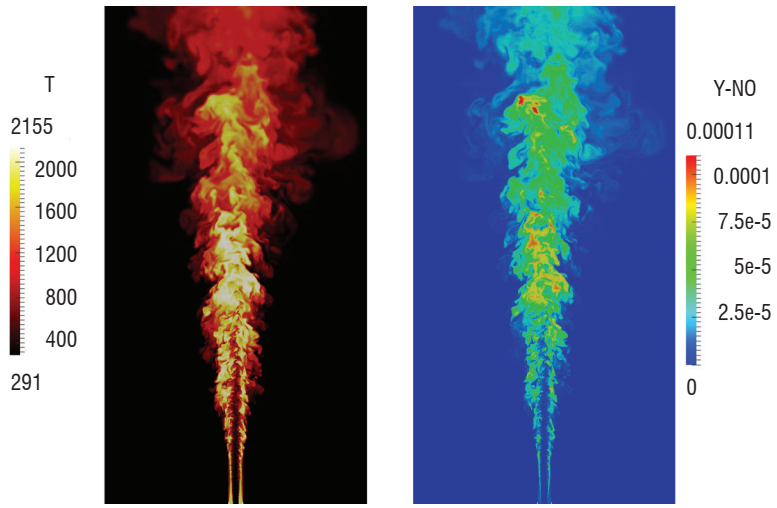


Figure 7 - Instantaneous temperature field (left) and instantaneous field of YN O (right), computed on a grid of 347 million mesh cells with a minimal resolution of 41 μm at the burner lip.

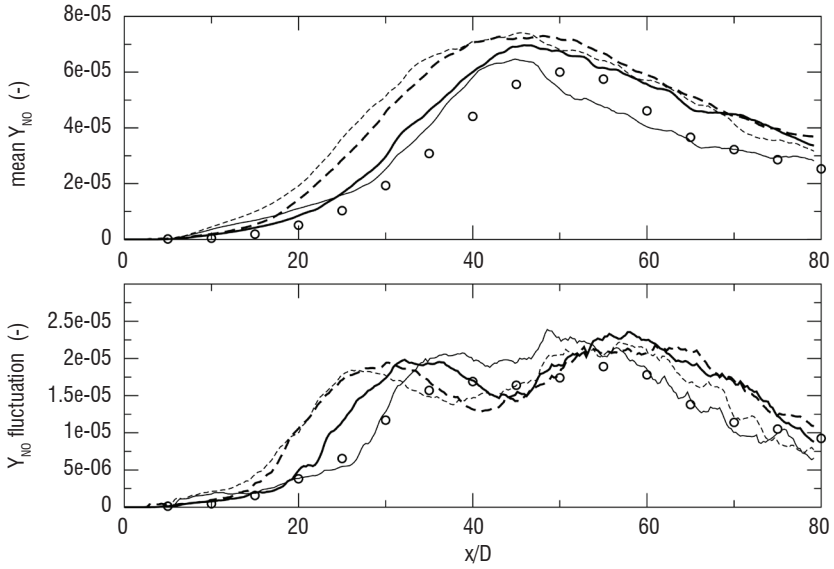


Figure 8 - Axial mean and rms NO mass fraction at the jet-fame centerline.
Symbols: experiment, Dashed lines: variable Lewis number modeling. Continuous lines: unity Lewis number modeling.
Resolution at the burner lip: 41 μm (Bold); 82 μm (Thin).

NOx

The heating of air in combustion systems produces nitric-oxides. This primary thermal source of NO features large characteristic time scales, at least much larger than the typical flow residence times of aero-engine combustion chambers [165, 166, 167]. NO levels are therefore always far from their chemical equilibrium reference state and predicting them is not an easy task. In addition, NO is also produced within the fuel oxidation thin layers, through a prompt nitric-oxide mechanism [168]. Even in a first approximation, this second mechanism cannot be neglected in accurate modeling, specifically in the fuel-rich zone of non- premixed flames in gas turbines [169, 170]. The numerical simulation of NO concentrations in this context has been the subject of multiple studies in both RANS and LES [171].

One of the major challenges in NO prediction is thus the large range of time scales that must be accounted for in the modeling, from fast fuel-oxidation, controlling the prompt mechanism, up to the slow thermal NO mechanism. Recently, an innovative approach called NOMANI (Nitrogen Oxide emission model with one-dimensional MANIfold) was dis- cussed [172], which includes the slow and fast chemical processes and which is well adapted to aeronautical engines, in which air is added downstream from the main combustion zone, in order to dilute the combustion products. In order ensure a precise estimation of the NO concentration in the flame front, as well as in the burnt gases, two progress variables are introduced in NOMANI. The first progress variable is derived from major carbon species, to monitor fuel oxidation. The second progress variable is based on the NO mass fraction and through variations in equivalence ratio, the NOMANI formalism provides a framework to account for secondary air-dilution. NOMANI is based on an a priori tabulation of the NO chemical sources and the effects of fluctuations unresolved by the mesh are accounted for using the PCM-FPI approach [173, 174].

NOMANI has been implemented in the flow solver YALES2 [175] and the SANDIA flame-D [176] was simulated to validate the NO prediction (see Figures 7 and 8). Since its preliminary validation on laboratory jet flames, NOMANI has been adopted by SAFRAN for NO prediction in the design loop of combustion chambers.

Conclusions

This article presented the modeling challenges encountered when performing LES of aeronautical combustion chambers. Issues relative to primary atomization, spray description, kerosene chemistry, combustion modeling and pollutant formation have been described. For each topic, we have given the current state-of-the-art within the context of Large Eddy Simulation. Several illustrative examples, representative of practical situations encountered in gas turbines, have been proposed. Future challenges are the fully coupled simulation, covering the interactions between all phenomena and all time and length scales involved, from the primary atomization at the fuel nozzle to the pollutant emitted at the exit of the combustion chamber ■

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Acronyms

RANS	(Reynolds Average Navier Stokes)
LES	(Large Eddy Simulations)
DNS	(Direct Numerical Simulations)
AMR	(Adaptive Mesh Refinement)
LDT	(Lagrangian Droplet Tracking)
DG	(Discontinuous Galerkin)
ACBMM	(Algebraic-Closure-Based Moment Methods)
QSSA	(Quasi Steady-State Approximation
PEA	(Partial Equilibrium Approximation)
DRG	(Directed Relation Graph)
QSS	(Quasi Steady State)
ILDM	(Intrinsic Low Dimensional Manifold)
F-TACLES	(Filtered TAbulated Chemistry for Large Eddy Simulation)
TSF	(Turbulent Stratified Flame)
LII	(Laser Induced Incandescence)
PIV	(Particle Image Velocimetry)
CARS	(Coherent Anti-Stokes Raman Spectroscopy)
NOMANI	(Nitrogen Oxide emission model with one-dimensional MANIfold)

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