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Impact of direct integration of Analytically Reduced Chemistry in LES of a sooting swirled non-premixed combustor

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ABSTRACT

Large-eddy simulation (LES) of a swirl-stabilized non-premixed ethylene/air aero-engine combustor experimentally studied at DLR is performed, with direct integration of Analytically Reduced Chemistry (ARC). Combined with the Dynamic Thickened Flame model (DTFLES), the ARC-LES approach does not require specific flame modeling assumptions and naturally adapts to any flow or geometrical complexity. To demonstrate the added value of the ARC methodology for the prediction of flame structures in various combustion regimes, including formation of intermediate species and pollutants, it is compared to a standard tabulation method (FPI). Comparisons with available measurements show an overall good agreement with both chemistry approaches, for the velocity and temperature fields. However, the flame structure is shown to be much improved by the inclusion of explicitly resolved chemistry with ARC. In particular, the ability of ARC to respond to strain and curvature, and to intrinsically contain CO/O_2 chemistry greatly influences the flame shape and position, as well as important species production and consumption throughout the combustion chamber. Additionally, since both chemistry descriptions are able to account for intermediate species such as OH and C_2H_2, soot formation is also investigated using a two-equations empirical soot model with C_2H_2 as the sole precursor. It is found that, in the present configuration, this precursor is strongly impacted by differential diffusion and partial premixing, not included in the FPI approach. This leads to a strong under-prediction of soot levels by about one order of magnitude with FPI, while ARC recovers the correct measured soot concentrations.

1. Introduction

Recent implementation of emission control regulations has resulted in a considerable demand from industry to improve the efficiency while minimizing the consumption and pollutant emissions of the next generation aero-engine combustors. Less expensive than Direct Numerical Simulations (DNS), Large Eddy Simulation (LES) is an attractive tool to address these issues with high accuracy at a reasonable computing cost, and is nowadays widely employed for the simulation of turbulent combustion in both academic and applied research (see, e.g., reviews of Pitsch [1] and Gicquel et al. [2], and references therein).

Accurate pollutant predictions rely heavily upon the fidelity of the chemistry description; however, the computation of combustion chemistry and its coupling with turbulent flows, a recent review of which can be found in Fiorina et al. [3], remains challenging in LES. One main reason is that fuel pyrolysis and oxidation proceed through complex and highly non-linear mechanisms involving hundreds of different chemical species over a wide range of characteristic length and time scales. As pointed out by Lu and Law [4] in their extensive review on the subject, the direct integration of such detailed chemistry in CFD applications like LES is not a viable path, because of excessive computational demands and numerical stiffness. Employing overly detailed chemical schemes for a specific application may not be desirable either, as this introduces a large number of reaction parameters, which individually contribute very little to the global flame behavior, while introducing possibly large uncertainties [5].

In practice, chemical kinetics in LES today is often taken into account through pre-tabulated laminar flame solutions based on detailed chemistry. As discussed by Peters [6], this method assumes that thermo-chemical evolutions in the composition/temperature space can be parametrized by a reduced set of variables. Usually, these include the mixture fraction, characterizing the degree of fuel and oxidizer mixing, and the progress variable, monitoring the progress of reaction towards chemical equilibrium. This approach is very attractive in that it does not require much CPU while enabling to retrieve virtually any

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thermochemical information of interest. Some recent techniques falling into that category include the flame-generated manifold (FGM) [7], the Flame Prolongation of ILDM (FPI) [8] or the Flamelet Progress Variable (FPV) [9] which have all been successfully coupled to various turbulence-chemistry interaction models to perform LES of complex geometries [10–13]. On the downside, simulations using tabulation are obviously very much dependent upon the type of canonical configurations chosen to build the look-up table (either premixed, partially-premixed or non-premixed) [14,15], even if recent efforts addressing this issue should be acknowledged [16,17]. Another main disadvantage of this approach is that the interactions between the flame and the flow are most often oversimplified. Indeed, taking into account complex phenomena such as turbulent, multi-species transport, dilution, heat losses or slow pollutant chemistry requires additional modeling efforts that can be far from trivial. Very often, additional parametrization variables are introduced, for which transport equations must be solved [18–20], resulting in additional unclosed terms and in an increase of the look-up table dimensionality. It is especially true in the context of soot modeling. Mueller et al. [21], for example, used a statistical Method of Moments in conjunction with a tabulated gas-phase chemistry description to investigate soot production in a real aeronautical burner, and their formulation required specific treatments to account for the loss of soot precursors from the gas-phase chemistry, and to include thermal radiation effects.

Introduced for example in Goussis et al. [22], another promising approach to model chemistry in LES is Analytically Reduced Chemistry (ARC). ARC is directly derived from detailed mechanisms, and accurately describes combustion phenomena by retaining only the main competing pathways and associated reactions. Typically, from 10 to 30 species and up to 500 reactions are considered, depending upon the hydrocarbon. ARC is nowadays easily derived to meet any type of requirements (combustion regime, operating range, stiffness), thanks to automated reduction tools [23,24] implementing efficient reduction techniques [25–28]. Associated with the ever increasing computational power, the use of ARC in LES has become very attractive. Jones et al. [29] were amongst the first to use ARC to investigate the flame structure in a relatively complex gaseous premixed burner, using a transported sub-grid PDF approach to model turbulent combustion. More recently, Bulat et al. [30] applied the same strategy to investigate CO and NO_x formation in an industrial gas turbine combustor. It is however of particular interest to combine ARC with a geometrical combustion model such as the Dynamically Thickened Flame (DTFLES [31]) approach, so as to benefit from the direct integration of the chemistry. A first successful attempt was made by Jaravel et al. [32] who employed ARC with DTFLES in the same configuration as Bulat et al. [30]. The authors also recently applied the same methodology in a two-phase flow burner, and obtained encouraging results [33].

To further assess the capacity of the ARC-DTFLES approach to accurately predict complex flame structures, it is used in the present study to investigate partial-premixing and gaseous chemistry involved in soot production. The configuration is a sooting swirled non-premixed gas turbine combustor burning ethylene with air, experimentally studied by Geigle et al. [34]. The objective is to perform a comprehensive investigation of the predictive capabilities offered by the ARC-DTFLES approach in a complex geometry where dilution and various combustion regimes are present, and to show how it may be used to predict soot levels. The LES is also performed with a standard tabulated approach (FPI [8]) in order to provide a comparison with a widely employed chemistry model. Finally, the ARC-DTFLES is applied to a second operating point in order to assess the flexibility of the approach.

The paper is organized as follows: the modeling approaches used for chemistry in this study are first reviewed in Section 2, and evaluated on relevant canonical one-dimensional problems. Next, the soot modeling strategy is described in Section 3. The experimental configuration is then introduced in Section 4 and the numerical strategy is presented in Section 5. Finally, in Section 6, the flow-field and flame structure obtained with both chemistry descriptions (ARC and FPI) are compared and discussed with respect to the experimental results. The analysis is completed with a discussion on soot precursors and soot predictions.

Table 1
Species contained in the ARC_18_C2H4NARA scheme.

Transported species	*QSS* species
N_2 H H_2 OH HO_2 H_2O H_2O_2 O O_2 CO CO_2 CH_3 CH_4 C_2H_2 C_2H_4 C_2H_6 CH_2O CH_2CO	C CH S-CH_2 T-CH_2 C_2H_3 C_2H_5 HCO HCCO CH_2CHO CH_3CHO C_2H_5O

2. Chemistry models

2.1. Development of the ARC mechanism

As discussed in the introduction, advanced reduction techniques have been developed to preserve the relevant chemical information of a detailed mechanism [22]. These techniques often complement each other and are therefore gathered in so-called "multi-step" reduction tools like YARC [24], employed in this study. The reduction with YARC is carried out in three steps, briefly presented hereafter.

First, a set of accuracy-preserving targets (flame speed s_l, auto-ignition time τ_{ig}) associated with a set of canonical zero- or one-dimensional configurations is prescribed. Next, based upon the results of these canonical cases, a skeletal reduction is performed where, following the formalism of Turanyi [35], unimportant species and reactions are removed from the original detailed mechanism. This step relies on the Directed Relation Graph with Error Propagation method (DRGEP). Finally, Quasi Steady State Approximation (QSSA) is formulated for a subset of species exhibiting small characteristic timescales, as identified by the Level of Importance (LOI) criterion [36]. This last step allows a considerable reduction of the stiffness from the mechanism. A full description of this procedure can be found in Pepiot et al. [37]. Note that to simplify the evaluation process, no quadratic coupling is allowed between QSS candidates.

Following this approach, an ARC has been derived for ethylene oxidation, starting from the detailed mechanism of Narayanaswamy et al. [38], originally composed of 158 species and 1804 irreversible reactions. The reduction is based on one-dimensional laminar premixed flames and zero-dimensional auto-ignition computations, in conditions representative of the studied configuration (T_f = 300 K and P = 3 bar). Targets consist of auto-ignition time (τ_{ig}), burnt gas temperature (T_b), laminar flame speed (s_l), main species equilibrium values, and specific intermediate species profiles (OH and C_2H_2). The resulting ARC is labeled ARC_18_C2H4NARA in what follows, and is comprised of 18 transported species and 11 QSS species, listed in Table 1.

2.2. Construction of the FPI table

The FPI-TTC tabulation method adapted to compressible solvers by Vicquelin et al. [39] is used. The look-up table is constructed from a collection of one-dimensional unstrained premixed laminar flames at the conditions of the target application (T_f = 300 K and P = 3 bar), computed with the solver Cantera [40] by assuming unity Lewis number for all species. The same detailed mechanism of Narayanaswamy et al. [38] employed for the ARC derivation is used. The flammability limits considered for the construction of the table are $0.4 < \phi < 3.0$. The table is parametrized with the mixture fraction Y_z based on the Bilger definition [41], and the normalized progress variable c based on the mass fraction of CO and