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Influence of chemical schemes, numerical method and dynamic turbulent combustion modeling on LES of premixed turbulent flames

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ABSTRACT

This paper describes Large Eddy Simulations of a turbulent premixed flame (the VOLVO rig) comparing Analytically Reduced Chemistry (ARC) with globally reduced chemistry for propane-air combustion, a dynamic Thickened Flame (TFLES) model with the usual non-dynamic TFLES model and a high-order Taylor Galerkin numerical scheme with a low-order Lax–Wendroff scheme. Comparisons with experimental data are presented for a stable case in terms of velocity and temperature fields. They show that going from two-step to ARC chemistry changes the flame stabilization zone. Compared to the usual non-dynamic TFLES model, the dynamic formulation allows to perform a parameter-free simulation. Finally, the order of accuracy of the numerical method is also found to play an important role. As a result, the high-order numerical method combined with the ARC chemistry and the dynamic TFLES model provides the best comparison with the experimental data. Since the VOLVO data base is used in various benchmarking exercises, this paper suggests that these three elements (precise chemistry description, dynamic parameter-free turbulent combustion model and high-order numerical methods) play important roles and must be considered carefully in any LES approach .

1. Introduction

The quest for a universal turbulent combustion model has been going on for a long time [1–4] but it has become more challenging in the last years. Today, turbulent combustion models are not only expected to provide reasonable estimates of mean heat release or temperature fields but also additional targets such as (1) pollutant emissions (NO*x* and CO for example) as well as soot, (2) possible combustion instabilities and noise level, (3) ignition and quenching phenomena. All these objectives must be satisfied for (4) liquid fuels, and (5) the detailed chemistry characteristics of real fuels must be included.

To satisfy these five objectives, the introduction of Large Eddy Simulation (LES) has offered a powerful approach [4–7] not because the subgrid LES models are better than their classical Reynolds Averaged (RANS) counterparts but because they are applied to a more limited part of the turbulence spectrum, while the rest of the unsteady activity is directly captured by the simulation. LES applied to combustion permits a better identification, at resolved scales, of the intermittency between fresh and burnt gases regions (where properties of turbulence, pollutant emissions, etc., are different) than RANS. However, what the last ten years have shown is that LES was only part of the solution. Many other ingredients remain necessary both on the physical and the numerical aspects to make LES predictive.

There are a few usual test cases for LES of reacting flows. For turbulent swirling flames, the PRECCINSTA chamber of DLR [8] has been computed many times [9–14]. Since PRECCINSTA is a swirled flame, many authors have started validations with an unswirled configuration and the so-called 'VOLVO' turbulent flame [15–17] has been used as a benchmark for turbulent combustion codes for a long time [18–20] for steady flames as well as for combustion instabilities [19]. Multiple solvers were applied for the VOLVO flames, leading to results which were all different [18] showing the lack of maturity of LES for turbulent flames. Considering that the VOLVO flames are fully premixed, gaseous flames,

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this indicates that major efforts are still required to address real flames such as those found in gas turbines for example.

The reasons why large discrepancies are observed for the VOLVO flames are not clear yet. Most solvers provide consistent, similar results for the cold flow in this setup, matching experimental data and demonstrating that the difficulties begin with combustion. Understanding which parts of the numerical strategy control the quality of the solution with combustion is a first but difficult step. Multiple potential sources of differences may be listed: (A) chemistry description, (B) flame/turbulence interaction model, (C) quality of the numerical solver, (D) boundary conditions, especially impedances at inlet and outlet which control the intensity of thermoacoustic modes, (E) wall numerical treatments, (F) wall temperatures and heat losses. The present work focuses on the first three sources (A) chemistry, (B) flame turbulence SGS models and (C) numerics.

Even if turbulent premixed flames can often be treated as thin interfaces, knowing whether the dynamics of these interfaces (response to small scale turbulence, to strain, to curvature) is really captured correctly for a given chemical scheme remains a daunting question for the LES community. Moreover, since objective (1) in real flames is to correctly capture all important species, LES chemical models must include more and more chemistry details. Knowing how the LES solution changes when a reasonably complex chemical scheme is used instead of a heuristic one or two-step scheme is the first objective of the present work. This objective is similar to the recent work of Zettervall et al. [20]. Note that it depends not only on the chemical scheme but also on the flame/turbulence interaction model (B) used in the LES. Here the TFLES (Thickened Flame model) is retained with either an usual non-dynamic (called static in the following) or a dynamic subgrid scale formulation. The third source (C) influencing the quality of LES results is the quality of the discretization scheme itself. This question is rarely discussed in the combustion community but is central in the aerodynamics community where the search for high-order methods has driven research for a long time. In the present study, a second and a third/fourth order method (space accuracy[1]) are compared: results show that turbulent structures and therefore the whole flame structure are indeed sensitive to the spatial accuracy of the discretization scheme, thereby explaining why different LES solvers often lead to different results even when all physical models are the same.

Of course, the three modeling sources affecting LES studied here (A-chemistry, B-SGS turbulent combustion model and C-numerics) are not the only ones controlling the quality of LES results. The present paper aims only at demonstrating that these three are important and that the quality of LES solutions cannot be investigated if these aspects are not properly considered.

The paper is organized as follows. First the description of propane-air chemistry (a two-step global scheme and the ARC formulation proposed by Pepiot et al. [22–24]) is presented in Section 2. Then, the two formulations, static and dynamic, of the TFLES model are described (Section 3). The convection scheme itself is presented in Section 4. Section 5 provides a description of the VOLVO setup and the stable combustion case retained for computations. Finally, Section 6 presents results, evidencing the influence of the subgrid scale model, the chemistry model and the convection scheme accuracy.

2. Chemistry description

In most turbulent flames, chemistry description can rapidly become an issue. The Volvo experiment is a usual benchmark for codes which ultimately will have to handle kerosene flames. Even if simplified chemical schemes (one or two steps) can be used for the premixed propane/air flames of the Volvo rig, going to more precise chemical schemes has become a necessity: today such options are readily maturing and for example, Analytically Reduced Chemistry (ARC) tools can produce chemical schemes that LES can fully resolve [23,24]. Here, two chemical schemes have been used to describe propane–air flames.

Table 1
Two-step reduced chemical mechanism for $C_3H_8 - Air$. Pre-exponential factor A_j and activation energies E_j are both in *cgs* units [19].

	A_j[cgs]	E_j[cgs]
Reaction 1	2.0×10^{12}	3.3×10^4
Reaction 2	-4.51×10^{10}	1.2×10^4

2.1. A two-step scheme for propane–air flames

The first scheme is a two-step scheme based on a fast oxidation reaction followed by a CO–CO_2 equilibrium. Six species are taken into account (C_3H_8, O_2, CO_2, CO, H_2O and N_2) and two reactions [19]:

$$C_3H_8 + 3.5O_2 \longrightarrow 3CO + 4H_2O \tag{1}$$

$$CO + 0.5O_2 \longleftrightarrow CO_2 \tag{2}$$

The reaction rates q_j follow an Arrhenius law:

$$q_1 = A_1 \left(\frac{\rho Y_{C_3H_8}}{W_{C_3H_8}}\right)^{0.9028} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.6855} \exp\left(\frac{-E_{a,1}}{RT}\right) \tag{3}$$

$$q_2 = A_2 \left[\left(\frac{\rho Y_{CO}}{W_{CO}}\right)^{1.0} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.5} - \frac{1}{K}\left(\frac{\rho Y_{CO_2}}{W_{CO_2}}\right)^{1.0}\right] \exp\left(\frac{-E_{a,2}}{RT}\right) \tag{4}$$

The pre-exponential constants A_j and the activation energies E_j are given in Table 1, and K is the equilibrium constant [25].

2.2. An analytically reduced scheme (22 species) for propane–air flames

The second method is based on the ARC approach. Using YARC reduction tools [22], the ARC chemical scheme is constructed from a skeletal mechanism proposed by Jerzembeck [26] using 99 transported species and 669 reactions. This skeletal scheme was derived from the LLNL detailed mechanisms for n-heptane [27] and iso-octane [28]. Laminar flames with an equivalence ratio in the range $\phi = 0.5$–1.6 are chosen as the sampled reference cases for the reduction process. The first step of the methodology is to discriminate unimportant species and reactions using the directed relation graph method with error propagation [29]. Then, suitable species for Quasi-Steady State Approximation (QSSA) are selected using the Level Of Importance criterion [30]. The resulting ARC chemical scheme (named ARC-22-12QSS in the following) treats 22 transported species and 12 QSS species (Table 2).

2.3. Comparison of two-step and ARC schemes on premixed laminar flames

Since the VOLVO experiment is fully premixed, a good method to compare chemical schemes is to apply them for premixed laminar flames. This is done here in terms of flame speeds and response to strain at atmospheric pressure. Adiabatic flame temperatures are not presented because they match very well for both

[1] The TTGC scheme used here [21] is fourth order accurate on regular unstructured grids and third order on arbitrary grids.