Combustion and Flame 192 (2018) 130–148

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Optimized single-step (OSS) chemistry models for the simulation of turbulent premixed flame propagation

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ARTICLE INFO

Article history:
Received 19 August 2017
Revised 14 October 2017
Accepted 26 January 2018

Keywords:
Premixed combustion
Turbulent flames
Single-step chemistry
Thermal expansion
Laminar flame speed
Flame thickness

ABSTRACT

A simple and efficient triple-optimization procedure (TOP) is introduced to determine single-step chemistry model parameters. The cornerstone of the proposed approach lies in the introduction of a fictive (or virtual) chemical species, the physical characteristics of which are set to recover some essential properties of combustion and flames. Special emphasis is presently placed on the capability of such a global kinetic scheme to recover three parameters that are recognized as the most influential in terms of turbulence–chemistry interactions and turbulent premixed combustion regimes. These parameters are (i) the burnt gases temperature T_b, which settles the value of the thermal expansion factor $\tau = (T_b - T_u)/T_u$, (ii) the propagation velocity S_L^0, which is mandatory to reproduce the flame dynamics, and (iii) the laminar premixed flame thickness δ_L^0. In practice, the thermochemical properties of the fictive species (hereafter denoted by A_Φ) are set to account for the impact of dissociation effects and partial oxidation of the fuel, i.e., presence of species other than H_2O and CO_2 in the burnt gases, which allows to recover a satisfactory estimate of T_b. The value of the pre-exponential factor associated to the single-step Arrhenius law is also optimized to reproduce the laminar flame propagation velocity. Finally, the transport characteristics are determined to recover a satisfactory estimate of the thermal flame thickness. The method is general in its principles and quite easy to implement. It is applicable to any couple of fuel and oxidizer. Attention is focused on the application of the method to any stoichiometry but it is also shown that the influence of both pressure and fresh reactants temperature can be recovered. The performance of the resulting optimized single step (OSS) chemistry models are assessed through a direct comparison with detailed chemistry results. Computations of one-dimensional laminar flames are performed with the OSS model using the `Cantera` software for a wide range of pressure levels, fresh reactant temperatures, and equivalence ratios. Obtained results do show that the flame propagation velocity is correctly reproduced for the whole range of parameters, with a maximum value recovered in the vicinity of stoichiometry, a decrease towards rich conditions, and a satisfactory pressure dependence. Burnt gases temperature as well as thermal flame thickness values are also in excellent agreement with those issued from the reference detailed kinetics models. The OSS model is then used to perform direct numerical simulation (DNS) computations of flame kernel growths in both laminar and turbulent conditions. The comparison of obtained OSS results with detailed chemistry computations further confirms the relevance and performance of the proposed methodology.

1. Introduction

Consideration of detailed chemistry effects has been early recognized as one of the most important challenges in computational combustion. This issue is especially critical for turbulent reactive flow simulation because of two principal causes: first (i) the numerical description of the turbulent flowfield is itself quite computational demanding and second (ii) the consideration of detailed chemistry within either the RANS or the LES modelling framework may rise some specific modelling difficulties. The transported PDF framework [1,2] may however offer an appealing way to circumvent the latter but this is at the price of some micromixing modelling difficulties and non-negligible additional computational costs. The last issue can be addressed through the *in situ* adaptative tabulation (ISAT), which accelerates reactive flow calculations [3,4]. The proposed strategy, i.e., ISAT, considers the whole detail of the chemical scheme but accounts, during an

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https://doi.org/10.1016/j.combustflame.2018.01.038

unsteady calculation, of all previously calculated states to map the chemistry. Nevertheless, despite the development of such efficient methodologies, it should be recognized that the use of detailed chemistry still suffers from too many severe limitations (including high computational costs, stiffness, etc.) to be routinely used in computational fluid dynamics (CFD) solvers. Several alternative procedures have been thus introduced to tackle the chemistry issue in turbulent reactive flows simulations.

The first alternative strategy is associated to tabulated chemistry models. It consists in proceeding with a direct *a priori* mapping of the detailed chemistry response onto a reduced number of characteristic variables such as progress variable, mixture fraction variable, characteristic strain-rate or scalar dissipation rate (SDR), with the last two quantities retained as relevant quantities to describe departures from chemical equilibrium. Most of these tabulation strategies have been developed under the laminar flamelet assumption. In the corresponding flamelet regime of turbulent combustion [5–7], the turbulent flame is thought of as a collection of local reactive elements that retain their identifiable steady laminar flame structure [8]. For non-premixed conditions, the foundations of such steady laminar flamelet models (SLFM) have been settled by Peters [9] with several extensions and refinements proposed since. For instance, some applications have been also based on unsteady flamelet calculations, see Barths et al. [10] and Pistch et al. [11]. In an attempt to go beyond fast chemistry regimes, some other tabulation strategies considered either the perfectly stirred reactor (PSR) or the partially stirred reactor (PaSR) as the elementary building blocks, see for instance references [12–15] for further details.

Based on the recognition that combustion thermochemistry is a non-linear process, the essential properties of which can be described in terms of an ODE system, i.e a large-dimension dynamical system, the characteristics of the integral solution (trajectory), i.e., manifolds and singularities, are of special interest. The intrinsic low dimensional manifold (ILDM) method of Maas and Pope [16,17] and the computational singular perturbation (CSP) method [18–20] exploit the same fundamental idea which is to suppress the fast modes. The consideration of a typical spectrum of chemical time scales indeed confirms that it covers a very large range of values, which may exceed seven orders of magnitude. The very fast time scales in chemical kinetics are usually responsible for equilibration processes: some elementary reactions are in partial equilibrium and some chemical species are in steady-state. This is in sharp contrast with slow chemical time scales such as those associated to nitric oxides (NO) formation. If we make use of this time scale disparity, it is possible to decouple the very fast time scales from the others, that is, local equilibrium can be assumed with respect to these fastest time scales. Besides the information gained from the mathematical study of stationary points, their stability or oscillatory behaviour, the proposed methods (i.e., ILDM and CSP) thus provide additional information on how, i.e., along which trajectory, the chemistry is approaching equilibrium. These methodologies gave birth to other approaches that are based on the consideration of the reaction-diffusion manifold (REDIM), see Bykov and Maas [21]. Finally, the coupling of such manifold-based strategies to standard tabulation methods also leads to flame-generated manifold (FGM) or flame-prolongated ILDM, i.e., FPI method [22,23] that have become very popular to proceed with turbulent combustion simulations. From a technical point of view, the generation and handling of the resulting lookup tables may however pose severe difficulties. In addition to this, and from a more fundamental point of view, the building block on which relies the tabulation – whatever it is based on the picture of a chemical reactor or a laminar flame structure – does restrict their applicability in terms of turbulent combustion regimes. Therefore, it is also very appealing to develop alternative methods where either global or reduced chemical schemes can be used directly in the reactive flow solver.

Reduced chemistry models have been early introduced in the literature [24–26]. Some essential information related to flame extinction, peak temperatures, and major species profiles can indeed be satisfactorily reproduced with the corresponding four- and five-step chemical mechanisms. For instance, recent efforts in this direction led to three- and four-step systematically reduced chemistry for hydrogen–air mixtures that are valid for a wide-range of hydrogen combustion problems [27,28]. The corresponding mechanisms have been successfully used to perform the numerical simulation of laboratory flames, see for instance [29], and the same reduction procedure has been also applied to the description of syngas combustion by the same group of authors [30,31]. In this respect, it is worth emphasizing that, from a mathematical (i.e., formal) point of view, the description of ignition problems requires at least the consideration of a two-step chemistry. This is indeed necessary to mimick the competition between the radical pool production and consumption rates, with the latter remaining dominant as long as the temperature remains below the so-called cross-over temperature, see for instance [32]. However, provided that attention is focused on the description of propagating premixed flames only, i.e., without any special consideration paid to the ignition problem, single-step chemistry is formally sufficient to reproduce the basic features of flame propagation similar to those obtained through detailed chemistry computations. In particular, as firmly established throughout the manuscript, the consideration of single-step chemistry suffices to reproduce the laminar flame characteristics that are involved in the classical set of non-dimensional parameters used to characterize the interaction between turbulence and combustion namely the laminar flame propagation velocity S_L^0 and thickness δ_L^0, plus the expansion factor τ. It is proposed herein to exploit this conclusion so as to optimize a parameterized single-step (i.e., global) chemistry description. It will be shown that the resulting OSS model allows to obtain a relevant estimation of the thermal expansion, laminar flame speed and thickness at a very moderate cost: four transport equations, a single reaction rate, and a tabulation of nineteen quantities.

Other studies have been recently conducted with similar targeted objectives. In particular, the laminar flame velocity S_L^0 can be reproduced for a large range of equivalence ratio through an optimization of the pre-exponential factor as early done by Vervisch et al. [33], Fernández-Tarrazo et al. [34], Reveillon [35] or Robin et al. [36]. More recently, Franzelli et al. [37] described a two-step chemistry model that satisfactorily recovers laminar flame propagation velocity and temperature in the burnt gases for a wide range of equivalence ratio Φ. It will be shown herein that similar performance can be achieved from the present optimized single-step (OSS) model. In practice, most of the available global mechanisms are valid only within a restricted range of equivalence ratio, and do not reproduce the laminar flame thickness or its internal structure evolution with Φ. Only some very recent (and seldom) efforts have been done to address these issues at the price of the use of genetic algorithms [38].

The present manuscript is organized as follows, the optimization procedure is described in the next section (Section 2). It includes three subsections that are devoted to (i) the fictive species thermochemical properties determination so as to reproduce the thermal expansion factor (i.e., burnt gas temperature), the restoration of (ii) laminar flame speed and (iii) laminar flame thickness from the automated determination of normalized pre-exponential factors and fictive species transport coefficients. The performance resulting from each optimization step is assessed in each subsection through comparisons with data issued from the detailed kinetic scheme of reference. In Section 3, the implementation of the resulting OSS model in the DNS solver `Asphodele` is used to