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Turbulent combustion modelling of a confined premixed jet flame including heat loss effects using tabulated chemistry ☆

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HIGHLIGHTS

- A turbulent combustion model based on the reaction progress variable is presented.
- An optimal choice of the reaction progress variable is proposed.
- Chemistry tabulation is based on laminar premixed flamelets including heat losses.
- The model is suitable for Reynolds-averaged Navier Stokes and large-eddy simulations.
- Good prediction capabilities are found for a turbulent premixed jet flame.

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ABSTRACT

The present work addresses the coupling of a flamelet database, to a low-Mach approximation of the Navier–Stokes equations using scalar controlling variables. The model is characterized by the chemistry tabulation based on laminar premixed flamelets in combination with an optimal choice of the reaction progress variable, which is determined based on the computational singular perturbation (CSP) method. The formulation of the model focuses on turbulent premixed flames taking into account the effect of heat losses, but it is easily extended to partially premixed and non-premixed regimes. The model is designed for applications in both, Reynolds-averaged Navier–Stokes (RANS) as well as large-eddy simulations (LES) and results for the two methods are compared. A priori analysis of the database is presented to demonstrate the influence of the reaction progress definition and the chemistry tabulation is validated against a one-dimensional premixed laminar flame. The validation of the turbulent case is performed using a turbulent premixed confined jet flame subject to strong heat losses, in which the model shows a good overall performance.

1. Introduction

The increasing energy demand and the yet more restrictive current emissions regulations are forcing the development of more efficient thermal systems and combustion engines [1]. As the main part of the global energy supply is still based on fossil fuels [2], the understanding of the combustion process is essential, since the chemical energy of the fuel is converted generally into thermal energy by combustion. Major challenges in the design of modern combustion engines include the reduction of pollutant emissions, increment of fuel flexibility, increasing cycle efficiency and flame stability [3]. To achieve these goals, an accurate description of the interaction of turbulence, chemical reactions and thermodynamics is required. In this context, the use of advanced numerical simulations is becoming a fundamental tool to provide detailed insights into the physical processes at relatively low cost. However, due to the different time and length scales existing in the combustion process, taking into account detailed chemistry in numerical simulations is still a challenge.

Although several attempts have been made to include detailed chemistry in numerical simulations of turbulent flames [4,5], these applications are still limited to relatively simple geometries and reduced reaction mechanisms due to the high computational cost.

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In particular, the inclusion of detailed chemistry of complex fuel blends for industrial applications is still prohibitive [6]. To overcome this difficulty, combustion models based on tabulated chemistry have been proposed to investigate the dynamics of turbulent flames at reduced computational cost [7–9]. Instead of solving transport equations for all chemical species involved in the reaction process, one or several scalars are used to represent the combustion chemistry in composition space [10]. Several reduction techniques have been proposed to separate fast and slow chemical scales. The intrinsic low-dimensional manifold (ILDM) was developed by Maas and Pope [11] to reduce chemical schemes for certain operating conditions. The CFI model (the abbreviation represents the controlling variables: reaction progress c, mixture fraction f and enthalpy scalar i) developed by Derksen [12] used a similar approach of reducing the chemical subspace by separating the different reaction time scales. The computational singular perturbation (CSP) method [13,12] was used to identify the species associated to fast and slow scales. These models yield good prediction capabilities in the high temperature range. However, non-equilibrium phenomena associated to the fast time scales, are not correctly reproduced. To overcome this disadvantage, the reduction method was extended to account for low-temperature regions and Lewis number variations by Gicquel et al. [6] in a model called flame prolongation of ILDM (FPI). Another well-established reduction method that is based on the solution of a steady, one-dimensional laminar flame for the generation of a manifold is the flamelet generated manifold (FGM) method proposed by van Oijen et al. [7]. These reduction methods have been successfully applied to premixed, non-premixed and partially premixed flames [14,7–9,15–17].

The combustion model presented in this paper, makes use of the FPI/FGM approach for chemistry tabulation and is based on laminar premixed flamelets. Scalar controlling variables are used to couple the tabulated chemistry to the flow solver in the combustion simulation. In the current framework of premixed, non-adiabatic combustion, a thermo-chemical database is generated by systematically varying the conductive heat losses at the burner inlet using a burner stabilized premixed flame. The database is then parametrized in terms of the normalized enthalpy and the reaction progress variable (RPV), which represents the state of reaction, storing transport properties and the RPV source term.

While the RPV is usually defined based on heuristic approximations and a priori knowledge of the flame characteristics, definitions based on optimization methods have been recently proposed [18,19]. In these approaches, constraints, like monotony and gradient thresholds, are formulated based on the chemical trajectories of the laminar flamelet. Subsequently, optimization tools are used to find the best definition of the RPV, which satisfies the constraints. In the current work, an optimized choice of the RPV definition is proposed making use of the computational singular perturbation (CSP) method [13,12]. The CSP method is applied to the laminar premixed flame computation prior to the tabulation process in order to obtain a RPV definition, in which the information about the different chemical time scales is incorporated. This results in an *optimized choice of the RPV* yielding to a more uniform distribution of the chemical subspace over the entire range and a reduction of the species derivatives in the thermo-chemical database. Furthermore, no a priori knowledge of the flame characteristics is required for the RPV definition.

An approach based on presumed shape probability density functions (PDF) is applied for chemistry-turbulence interaction. The proposed model is applied to address high-fidelity numerical simulations in the context of large-eddy simulation (LES), but is also designed to provide acceptable results for industrial-type applications for Reynolds-averaged Navier–Stokes (RANS) simulations. Therefore, in the course of the paper, the model definition is discussed with a view to the differences between RANS and LES, and finally the results of the two formulations are compared for a premixed turbulent jet flame.

The proposed combustion model is implemented in the High-Performance Computing (HPC) multi-physics code Alya [20]. Alya is based on the Finite Element method using the Variational Multiscale Stabilization (VMS) approach [21] and is designed for large-scale parallel applications [22]. Even though the current work focuses on premixed combustion and the influence of heat losses, the model formulation can be extended to partially premixed and diffusion flames by the addition of the mixture fraction as an additional controlling variable. A special computation of the temperature based on a polynomial expression is used, which allows the application of the model in a low-Mach framework as well as for fully compressible flows.

In the current paper, the proposed combustion model and the implementation in the HPC finite element code Alya is validated for the turbulent premixed jet flame that has been experimentally investigated by Lammel et al. [23]. The conditions under investigation correspond to a confined lean premixed methane/air flame with equivalence ratio of 0.71. The burner is operated at ambient pressure with a mixture preheated up to 573 K. The same test case has been used for numerical validation by other authors and the main results are subsequently summarized. Donini et al. [24] investigated the influence of heat loss using a FGM implementation in the commercial CFD code CFX in combination with a RANS approach. It was shown that for the current test case the addition of heat losses in the combustion model is essential to correctly predict the flame structure. Fancello et al. [25] performed a LES simulation of the premixed jet flame using the FGM model in OpenFOAM and Proch and Kempf [26] used the test case to validate different heat loss modelling approaches for FGM in the context of LES. The present work is a contribution to the modelling of the combustion dynamics of this test case, in which RANS and LES are systematically compared using the same turbulent combustion model and numerical methods.

The current paper is organized as follows. In Section 2.1, a detailed description of the chemical database calculation is given followed by the mathematical modelling employed for turbulent calculations in RANS and LES (Sections 2.2 and 2.3). In a first testing step, the formulation of the combustion model is compared against a detailed chemistry computation for a one-dimensional laminar premixed flame in Section 3. Subsequently, in Section 4 the model performance for RANS and LES is evaluated using a turbulent premixed jet flame subjected to heat losses.

2. Mathematical modelling

This section describes the mathematical modelling used in the current work to obtain the solution fields for RANS and LES. The proposed combustion model is described in detail. Focus is set on the procedure of the chemistry tabulation and the transport equations that are used to represent the combustion chemistry in the numerical calculation. Moreover, the utilized governing equations of fluid dynamics are presented in the low-Mach framework with emphasis on the differences between RANS and LES.

2.1. Chemistry tabulation

The proposed combustion model is based on the generation of a thermo-chemical database from a detailed chemistry calculation of a one-dimensional premixed flame. This procedure reduces the stiffness of the reacting flow simulation and is performed in a pre-processing step. In this section, the tabulation procedure is

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