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A priori Tabulation of Turbulent Flame Speeds via a Combination of a Stochastic Mixing Model and Flamelet Generated Manifolds[5]

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A priori Tabulation of Turbulent Flame Speeds via a Combination of a Stochastic Mixing Model and Flamelet Generated Manifolds

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Abstract

In this paper we propose a technique for *a priori* turbulent flame speed tabulation (TFST) for a given parameter space in standard combustion-regime diagrams. It can be used as a subgrid-scale (SGS) model in Large Eddy Simulation (LES). In a first step, stationary laminar flamelets are computed and stored over the progress variable following the ideas of flamelet generated manifolds (FGM). In a second step, the incompressible one-dimensional Navier-Stokes equations supplemented by the equation for the progress variable are solved on a grid that resolves all turbulent scales. Additionally, turbulent transport is implemented via the linear eddy model (LEM). The turbulent flame structures are solved until a statistically stationary mean value of the turbulent flame speed has been reached. The results are stored in a table that could be used by large scale premixed combustion models, e.g. front tracking schemes. Results are compared to an algebraic model and to direct numerical simulations (DNS).

Keywords: turbulent premixed combustion, flame structures, linear eddy model, flamelet generated manifolds, turbulent burning speed tabulation

Contents

1 Introduction

Due to the interaction between many different time and length scales, turbulent premixed combustion simulation remains a challenging task. Whereas the largest turbulent scales and the slow chemical processes are resolvable, the small scale turbulence/chemistry interaction often has to be modelled. Therefore, the reactive Navier Stokes equations are filtered, dividing the original solution into resolved and unresolved parts, where the latter needs closure. This is commonly done using parameterizations that relate the unresolved parts to the resolved field. For example, the turbulent flame speed, s_t, is an important quantity [13], that is used in many approaches to premixed combustion modeling, e. g., level set methods, flame surface density models, and progress-variable type approaches [4, 14, 20]. There are different possibilities to evaluate this property. The simplest and perhaps least physical is a simple algebraic expression, where often s_t is a function of the unburnt (indicated by subscript u) thermodynamic state and turbulent fluctuations, say

$$s_t = f(u', \boldsymbol{Y}_u, T_u, p_u), \tag{1}$$

where $u', \boldsymbol{Y}, T, p$ are the velocity fluctuation, species mass fraction, temperature and thermodynamic pressure, respectively. Additionally, curvature and stretch effects can be taken into account.

The turbulent flame speed might as well be extracted from stand-alone computations of detailed turbulent flame structures [1, 15].

More recent methods use so-called superparameterizations to determine s_t. Here a one-dimensional microstructure evolution for turbulence chemistry interaction, e.g. [16], is forced by the resolved solution. Suitable integrals over the microstructure yield some of the needed closure terms like the turbulent flame speed. However this procedure is done "online", increasing the costs of such a computation considerably. Even for (stand-alone) one-dimensional calculations of turbulent premixed flames using detailed chemistry and the Linear Eddy Model (LEM [9]) for turbulent transport, the effort is quite high [11, 15].

In this paper, we propose a technique of *a priori* tabulation of s_t for a given reactive setup, e.g., geometric scales, fuel, equivalence ratio, and so on. It can be used as SGS model for LES. The different s_t for the table are computed by evolving one-dimensional turbulent flame structures to a statistically steady state. The steady state assumption is tested with unit root tests and looking at the convergence of the mean. In the flame structure computation we use LEM for the turbulent transport and the idea of Flamelet Generated Manifolds (FGM) [19] for the chemistry tabulation. Both are linked to an implicit solver for the one-dimensional Navier-Stokes equations [8].

As long as the smallest turbulent eddies do not enter the reaction zone, (laminar) chemistry and turbulence can be treated separately. For the chemistry we apply FGM [19] using the code from [11]. In a first step we compute steady one-dimensional laminar flamelets with detailed chemistry and tabulate the flame structure as a function of a suitable progress variables, e. g. CO_2 for a methane air mixture. Additional parameters for tabulation depending on their physical relevance could be stoichiometry, enthalpy, or flame stretch, which changes the laminar burning velocity. In DNS-FGM a correct influence of stretch on the burning velocity was found in Bastiaans et al. [2]. Here stretch effects are not explicitly taken into account.

In the second step we solve the zero Mach number equations for mass, momentum, energy, and progress variable in a one-dimensional domain resolving all spatial and temporal scales. Turbulent advection is implemented using the stochastic LEM. Species mass fractions are uniquely determined by mapping between the progress variable and the pre-calculated FGM of step one. The calculations of step two are performed until a statistically stationary value of s_t has been reached. The extension of our LEM/FGM ansatz to account for stretch effects is currently investigated and will be published elsewhere.
This paper is organized as follows. In the next section, we outline our modeling approach. In section 3 results for turbulent premixed flames for different equivalence ratios and turbulence intensities are presented. These results are compared with currently used algebraic models and DNS. The paper ends with conclusions on the approach and an outlook for further investigations.

2 Model Formulation

Our modeling approach consists of a combination of different stand-alone models, where each model tries to reduce the complexity and cost of turbulent reactive multi-dimensional flow computations. The main steps are (i) constructing a FGM table by computing a sequence of laminar flames to a steady state, (ii) computing a sequence of turbulent flame structures using LEM and the FGM results from (i), (iii) extracting the turbulent burning speed for each run when convergence of the mean is reached, and (iv) building the turbulent data base.

2.1 Flamelet generated manifolds

To make the sequence of turbulent flame structure computations feasible, we apply the flamelet generated manifold (FGM) method [19] to obtain chemical source terms and local mass fraction values. FGM can be considered as a combination of the flamelet approach and the intrinsic low dimensional manifold (ILDM) method [10] and is similar to the flame prolongation of ILDM, FPI, introduced in [6]. FGM is applied similar to ILDM. However, the data base is not generated by applying quasi-steady-state relations for chemical source terms, but by solving a set of one-dimensional convection-diffusion-reaction equations to a steady state of a laminar flame structure. The main advantage of FGM is that diffusion processes, which are important between the preheat zone and the reaction layer, are taken into account. This leads to an accurate method for premixed flames that uses fewer controlling variables than ILDM. The manifold used in this paper is based on a methane/air kinetic mechanism with 16 species and 36 reactions taken from [12]. The extension of the idea to more complicated mechanisms is straightforward [5].
In order to generate the manifolds in step (i), we solve the variable-density zero-Mach-number equations in one spatial dimension on a regular grid. The balance equations for species mass fractions Y_s and temperature T are

$$\rho\frac{\partial Y_s}{\partial t} + \rho u\,\frac{\partial Y_s}{\partial x} = -\frac{\partial j_s}{\partial x} + M_s\,\dot{\omega}_s, \tag{2}$$

$$\rho c_p\frac{\partial T}{\partial t} + \rho u c_p\,\frac{\partial T}{\partial x} = -\frac{\partial q}{\partial x} - \sum_s j_s\,\frac{\partial h_s}{\partial x} - \sum_s h_s\,M_s\,\dot{\omega}_s, \tag{3}$$