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A generalized flamelet tabulation method for partially premixed combustion

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ABSTRACT

A flamelet tabulation method for partially premixed flames is proposed, in which partially premixed flamelets are incorporated as the archetypal flamelet elements. This method considers triple flame structures with both the partial premixing of fuel in the oxidizer side and the partial premixing of oxidizer in the fuel side, by replacing the pure-air and pure-fuel in the counterflow diffusion flame with a range of fuel-lean and -rich mixtures, respectively. The thermo-chemical quantities in the partially premixed flamelet are stored in a four-dimensional flamelet library as a function of the mixture fraction Z, describing the mixing process, the reaction progress variable Y_{PV}, describing the progress of reactions, and the trajectory variables Y_F and Y_O, characterizing the partial premixings of fuel and oxidizer, respectively. The performance of the proposed partially premixed flamelet tabulation (PPFT) method is evaluated through both *a priori* and *a posteriori* tests on laminar tribrachial flames with different mixture fraction gradients. The PPFT results are compared with those from a premixed flamelet tabulation (PFT) method and a diffusion flamelet tabulation (DFT) method. It is found that the combustion-mode-sensitive species such as CO and H_2 can be accurately predicted by the PPFT method for both the low and high mixture fraction gradient flame cases, which cannot be well predicted by the PFT and DFT methods.

1. Introduction

In practical combustion systems, partial premixing of reactants is commonly observed [1–4]. It is of significant practical interest to develop combustion models that can accurately predict the phenomenon of partially premixed flames (PPF). Among the combustion models proposed for PPF, the flamelet tabulation models have been widely used (e.g., Refs. [3–7]) because they can take detailed chemistry mechanism into account without high computational cost. In the flamelet models, a chemistry table containing all of the interested thermo-chemical quantities is often pre-calculated by solving prototype one-dimensional (1D) laminar flames. For example, the steady laminar flamelet (SLF) model [8] and the flamelet/progress variable (FPV) approach [9,10] assume that combustion chemistry can be mapped by a collection of 1D counter flow diffusion flames at various strain rates, while the premixed-based flamelet models such as the flame prolongation of intrinsic low-dimensional manifolds (FPI) [11] and flamelet-generated manifolds (FGM) [12] assume that the thermo-chemical state can be mapped by a collection of 1D freely propagating premixed flames at various equivalence ratios. Recent review works on FPV and FGM modelling can be referred to [13,14].

There are inherent limitations using premixed flamelets to tabulate diffusion combustion or using diffusion flamelets to approximate premixed combustion. This is because the impact of interactions between iso-equivalence-ratio surfaces are neglected in the premixed flamelets, whereas the propagating premixed flames are *a priori* not included in the diffusion flamelets. Nguyen et al. [15] observed clear differences in tabulated trajectories between premixed and diffusion flamelets. To remedy such deficiencies, they derived a multidimensional flamelet model, in which a projection of the full set of unsteady-mass-conservation species and energy balance equations is solved [15]. Scalar dissipation rates for mixture fraction and reaction progress variable appear in the projected low-dimensional equations, which need to be modeled. A similar method called REDIM (REaction-DIffusion Manifolds) was proposed by Bykov and Maas [16]. With proper selection of the initial conditions for the manifold evolution equations, the REDIM method was shown to be able to describe partially premixed flames [17].

The main deficiency of the widely used tabulation methods (e.g., SLF, FPV, FPI and FGM) is that they depend on flamelets assuming a single combustion mode. To overcome this weak point,

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some researchers [3–6] linearly combined the diffusion-flame-based flamelet (e.g., SLF, FPV) and premixed-flame-based flamelet (e.g., FPI, FGM) in separate chemistry tables in order to incorporate multi-combustion modes of partially premixed flames. These models are somewhat straightforward in a pure mathematical sense and improved simulation results can be obtained compared to the single-mode combustion model results. However, it should be noted that the diffusion-flame-based flamelet and premixed-flame-based flamelet represent asymptotic limits of combustion modes. Therefore, a blending procedure is physically not justified. Instead of blending combustion-mode-specific models in the local cell, Wu et al. [18] developed a so-called Pareto-efficient combustion (PEC) framework to dynamically utilize different combustion models in different combustion regions, optimizing the computational cost and simulation accuracy for interested quantities over the entire computational domain. The capability of the PEC framework has been evaluated in a laminar tribrachial flame [18].

A more reasonable tabulation method for PPF is to generate chemistry table based on partially premixed flamelets. Inspired by this idea, Franzelli et al. [7] replaced the pure-fuel in the counterflow diffusion flame with the fuel/air mixture. The partially premixed flamelet library was generated for different values of equivalence ratio and strain rate. This new tabulation method was evaluated on a referred kerosene counterflow spray flame with an *a priori* test. They found that this new tabulation method describes the flame structure more satisfactorily than the classical techniques based on single archetypal flamelets [7]. The improvement of this new tabulation method can be attributed to the fact that the partial premixing of oxidizer in the fuel side is considered in the chemistry table, by adding oxidizer to the fuel side of the archetypal flamelet. However, the partial premixing of fuel in the oxidizer side also happens quite often in configurations such as lifted flames. Thus, it is necessary to reconsider a more general flamelet model for partially premixed flames.

In the present paper, a generalized flamelet tabulation method for partially premixed flames is proposed, in which the triple flame structures with both the partial premixing of fuel in the oxidizer side and the partial premixing of oxidizer in the fuel side are considered. Two new trajectory variables are introduced to characterize the partial premixings of fuel and oxidizer explicitly. The newly proposed tabulation method is evaluated through both *a priori* and *a posteriori* tests on laminar tribrachial flames with different mixture fraction gradients. The results of the generalized flamelet tabulation method are compared with the reference solutions calculated with detailed chemistry, and those from a premixed flamelet tabulation (PFT) method, and a diffusion flamelet tabulation (DFT) method.

The remainder of this paper is organized as follows. In Section 2, the numerical modeling approach is presented. The numerical implementations are provided in Section 3. Results and discussion are given in Section 4. The paper ends up with conclusions.

2. Numerical methods

2.1. Detailed chemistry numerical simulations

Detailed chemistry numerical simulations are conducted to provide the reference solution. The governing equations for mass, momentum, species mass fraction and total enthalpy are solved in the reference case without filtering or averaging [19],

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho u_j\right)}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2\mu}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right] \tag{2}$$

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial (\rho u_j Y_k)}{\partial x_j} = -\frac{\partial J_k}{\partial x_j} + \dot{\omega}_k, \quad k = 1, 2, \ldots, N \tag{3}$$

$$\frac{\partial (\rho H_e)}{\partial t} + \frac{\partial (\rho u_j H_e)}{\partial x_j} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_i} - \sum_{k=1}^{N} J_k H_{e,k}\right) \tag{4}$$

where u_i is the velocity in the ith direction, ρ is the density, which is calculated from the state equation for ideal gas, μ is the dynamic viscosity, p is the static pressure, δ_{ij} is the Kronecker delta function, Y_k is the mass fraction of species k, J_k is the diffusion flux of species k, which will be given shortly. $\dot{\omega}_k$ is the reaction rate of species k, which is calculated by the finite rate chemistry model with the GRI-Mech 3.0 chemical reaction mechanism (53 species, 325 reactions) [20]. N is the number of species to be transported. The species mass fraction of N_2 is calculated by subtracting other species mass fractions from unity. H_e is the specific total enthalpy, λ is the heat conductivity, T is the gas temperature. Note that the viscous dissipation, radiation and the Soret and Dufour effects in the enthalpy equation are all neglected for simplicity.

In the present work, the diffusion flux J_k is modelled with the species diffusion velocity $V_{D,k}$ and the correction velocity V_C [19],

$$J_k = V_{D,k} + V_C \tag{5}$$

$V_{D,k}$ and V_C are respectively calculated according to the Fick's law and the model by Coffee and Heimerl [21],

$$V_{D,k} = -\rho D_k \frac{\partial Y_k}{\partial x_i}, \quad V_C = Y_k \sum_{m=1}^{N} \frac{\rho D_m \partial Y_m}{\partial x_i} \tag{6}$$

where D_k (or D_m) is the mass diffusivity of species k (or m), which is calculated as $D_k = \lambda/(\rho C_p)$ under the assumption of unity Lewis number. In the present study, unity Lewis number flames are considered since unity Lewis number assumption excludes the model uncertainties and simplifies the analysis of the simulation results. Previous studies [22,23] showed that the differential diffusion (non-unity Lewis number) effects result in additional tangential diffusion terms in the flamelet equations, which may have non-negligible effects for certain flames where the transport of species and temperature along mixture fraction isosurfaces is comparable with that in the mixture fraction gradient direction. However, in the limit of unity Lewis number, the effects of flame curvature, preferential transport and curvature induced multidimensional effects can be neglected [24–26]. Therefore, the unity Lewis number assumption has been widely used in flamelet tabulation models (e.g., Refs. [6,12,18]). It should be, however, noted that neglecting differential diffusion effects in the tabulated database may introduce biases in the flame speed prediction.

2.2. Tabulation methods

The tabulation method proposed in this work is based on partially premixed flamelets, referred to as PPFT, considering the triple flame structure and the partial premixings of fuel and oxidizer. The PPFT chemistry table is generated by injecting a fuel-lean premixed mixture against a fuel-rich premixed mixture for different values of equivalence ratio ϕ and strain rate a, as schematically shown in Fig. 1. The equivalence ratio on the lean side varies from the stoichiometric condition ($\phi_l = 1$) to the pure-air ($\phi_l = 0$) while