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Reactive parametrized scalar profiles (R-PSP) mixing model for partially premixed combustion

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ABSTRACT

Probability density function (PDF) methods are especially suited for turbulent combustion calculations, since the averaging of the reaction source term in the governing equation poses no closure problem. Molecular mixing and computing thereof in the presence of chemical kinetics, however, remains a major modeling challenge; not only for PDF methods.

In this work we present a new model for partially premixed combustion based on the joint statistics of mixture fraction, scalar dissipation rate and a burning indicator, which is used to evolve notional fluid particles in mixture fraction-reactive scalar space (e.g., enthalpy). Therefore, the parameterized scalar profile (PSP) mixing model was extended for reactive scalars. As in the PSP mixing model for inert scalars, each fluid particle is associated with a representative profile in physical space. Different than in the standard PSP model, the reactive profiles get modified by chemical reactions. The decision whether a fluid particle is reacting or not is based on a burning indicator, the local scalar dissipation rate and the profile boundaries. The burning indicator accounts for the flame propagation in the partially premixed environment and controls extinction and re-ignition; together with the scalar dissipation rate. The solutions of the reaction–diffusion equation for different scalar dissipation rates is used to determine the state of the embedded flame associated with a reacting particle, which allows to construct reactive scalar profiles and on the other hand pure diffusion is assumed for extinct particles.

The new combustion model was validated with the Sandia flame F data and comparisons demonstrate its ability to account for the relevant phenomena in partially premixed flames.

1. Introduction

There exists a great demand for reliable and accurate combustion models, since the direct solution of the governing conservation laws with reaction kinetics is unfeasible for most practical applications. Both, experiments and direct numerical simulations (DNS) are, however, extremely valuable to improve our understanding of the physical phenomena related to turbulence–reaction interactions and to develop better combustion models.

A possible and attractive way to simulate turbulent reactive flows is based on transported probability density function (PDF) methods [1] in the context of Reynolds averaged Navier–Stokes. One major advantage of PDF methods is that a higher level of closure is achieved than with classical RANS methods and that they are computationally much more efficient than large eddy simulation (LES), which can also be used together with a PDF closure (FDF methods) [2,3]. For example, in joint velocity-composition PDF methods turbulent convection and reaction source terms appear in closed form [4]. Furthermore, the full one-point one-time joint statistics of these quantities is available and can be employed for better modeling of e.g., molecular mixing coupled with reactions. A recent review of PDF methods can be found in [5].

Provided the chemical reaction mechanism is known, the reaction source term can be computed by direct integration without additional assumptions. In general, however, this is very costly due to the typically large and stiff system of nonlinear ordinary differential equations (ODEs), which has to be solved [6]. Therefore, different techniques were developed to reduce the cost for the computation of the chemical source terms. One approach consists in reducing the number of influential species and reactions. To achieve this, Peters [7] introduced quasi steady state assumption (QSSA) for intermediate species. Maas and Pope [8] devised the intrinsic low-dimensional manifolds (ILDM) method, which also aims at reduced reaction mechanisms. Later, Bykov and Maas [9] proposed reaction–diffusion manifolds (REDIM), which account for the influence of molecular diffusion on the chemical reactions. Another approach by Pope [10], who developed the in situ adaptive tabulation (ISAT) method, can be regarded as an algorithmic trick to reduce the overall cost by replacing some of the expensive time integration steps with simple lookup operations from tables built

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during the simulation. The ISAT algorithm proved to be extremely effective, especially if the accessed domain in the high dimensional scalar space lies on a low dimensional manifold. The combination of PDF methods with direct integration, reduced mechanisms or ISAT was successfully applied to simulate many turbulent reactive flows, e.g., Cao and Pope [11], Raman et al. [12], Lindstedt et al. [13], Tang et al. [14], Merci et al. [15] and Nooren et al. [16].

However, for an accurate and general description of the embedded flame structures in a turbulent flow field, an exact but isolated integration of the reaction source term is not sufficient. Instead, the fully coupled convection–diffusion–reaction problem has to be considered. Motivated by this fact, Peters introduced the laminar flamelet concept [17], which has been very successful in particular for non-premixed combustion [18–22]. This paper deals with the case of partially premixed combustion, where local extinction can occur due to increase of the scalar dissipation rate (mainly induced by high strain) and local re-ignition due to propagation of embedded quasi laminar triple flames. Based on a constructed fine-scale picture of the scalar fields, an efficient combustion model is proposed, which accounts for these effects.

To model partially premixed flames, one can either start from a premixed or a non-premixed perception. Bradley et al. [23,24] followed the first approach and successfully applied a premixed combustion model with imposed flammability limits. Later, they extended the model and allowed for premixed flame quenching due to strain. On the contrary, Sanders and Lamers [25] used diffusion flamelets and modeled extinction as a function of flame stretching. Both models were applied to simulate the canonical lifted non-premixed jet flame and could correctly predict the linear dependency of lift off height on the fuel jet velocity. Müller et al. [26] took a slightly different route and calculated scalar fields of a level set function and the mixture fraction. The level set function describes the location of the flame front, whereas the mixture fraction is a passive mixture equivalence ratio indicator. An important modeling issue of this approach is their specification of the reaction source term in the mean level set equation. This includes the turbulent flame speed depending on the laminar flame velocity, a term accounting for partial premixing and a flame quenching term based on the scalar dissipation. With this model they were able to compute the correct lift off height. More recent approaches use a reaction progress variable together with a flamelet model. Such combustion models are applied for instance in multiple mapping conditioning (MMC) methods [27] or in the context of subgrid combustion models in LES codes by Domingo et al. [28], Pierce and Moin [29], Vervisch and Domingo [30] or Ihme and Pitsch [31,32]. The main task there is to obtain accurate statistical information for different scalar quantities, i.e., mainly joint information of progress variable, mixture fraction and scalar dissipation rate.

To compute the joint statistics of progress variable, mixture fraction and scalar dissipation rate, PDF methods are extremely attractive. This however implies the need for not only an accurate mixing model, but also a consistent closure for the scalar dissipation rate. In this work, we further develop the reactive IEM mixing model by Hegetschweiler et al. [33], which involves a burning indicator and a modified flamelet approach. The basic idea of the new model is to treat the influence of mixing and reactions together. Therefore statistical representative laminar profiles of mixture fraction and reactive scalars are considered, which are embedded in the turbulent flow field. The idea to statistically describe mixing in turbulent flows by laminar one dimensional scalar profiles was first suggested and developed by Meyer and Jenny [34,35] (parametrized scalar profile or PSP mixing model).

In their work, a parametrization based on sinusoidal profiles was introduced and proved to be very predictive for inert multicomponent mixing. For reacting scalars, on the other hand, a more general profile parametrization is required, e.g., as suggested in this paper. To capture local extinction it is a major advantage that the PSP mixing model also provides the scalar dissipation rates without additional closure assumption. Local re-ignition occurs with a modeled ignition probability. Validation studies and comparison with experimental data of Sandia flame F show good agreement for first and second order statistics, also compared with the previous work of Pope [10] and Hegetschweiler et al. [33]. Additionally scatter plots and joint PDFs of mixture fraction and temperature are presented, which are also in reasonable agreement with experimental findings.

In the following section, the basic concept of transported PDF methods is outlined. In Section 3, first a short review of the PSP mixing model is presented, followed by an explanation of the new reactive PSP model. Validation results are discussed in Section 4 and finally, conclusions are given in Section 5.

2. Transported joint PDF method

In this section we consider the one-point one-time joint PDF $f(\boldsymbol{V},\boldsymbol{\Psi},\theta;\boldsymbol{x},t)$ of velocity $\boldsymbol{U}$, composition vector $\boldsymbol{\Phi}$ (including mixture fraction $Z=\Phi_1$ and sensible enthalpy $h_s=\Phi_2$) and turbulence frequency ω. $\boldsymbol{V}$, $\boldsymbol{\Psi}$ and θ are the sample space variables of $\boldsymbol{U}$, $\boldsymbol{\Phi}$ and ω, respectively. In case of the R-PSP model, the profile boundary values $h_s^{\pm}$ and $Z^{\pm}$ are also part of the composition vector. In the case of reactive turbulent flows with large density variations, it is beneficial to work with the mass density function (MDF) $\mathscr{F}(\boldsymbol{V},\boldsymbol{\Psi},\theta,\boldsymbol{x},t)$ instead, which is defined as

$$\mathscr{F}(\boldsymbol{V},\boldsymbol{\Psi},\theta,\boldsymbol{x},t)=\rho(\boldsymbol{\Psi})f(\boldsymbol{V},\boldsymbol{\Psi},\theta;\boldsymbol{x},t). \tag{1}$$

Note that here the low Mach number approximation is made, which means that the density depends only on a reference pressure and the composition vector $\boldsymbol{\Phi}$ and not on pressure fluctuations. A transport equation for the MDF can be derived by standard methods, see e.g., Pope [4], and becomes

$$\begin{aligned}\frac{\partial\mathscr{F}}{\partial t}+\frac{\partial \boldsymbol{V}_i\mathscr{F}}{\partial x_i}=&-\frac{\partial}{\partial V_i}\left[\left\langle\frac{\mathrm{D}U_i}{\mathrm{D}t}\middle|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right]\\&-\frac{\partial}{\partial\Psi_\alpha}\left[\left\langle\frac{\mathrm{D}\Phi_\alpha}{\mathrm{D}t}\middle|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right]\\&-\frac{\partial}{\partial\theta}\left[\left\langle\frac{\mathrm{D}\omega}{\mathrm{D}t}\middle|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right].\end{aligned} \tag{2}$$

This equation describes the temporal evolution of the MDF in physical-, composition- and turbulence frequency space. Note that repeated indexes imply Einstein's summation convention and angle brackets denote common Reynolds averages. The first two substantial derivatives on the right hand side can be substituted by the corresponding expressions from the Navier Stokes (NS) and the composition conservation equations, respectively, and we obtain a MDF transport equation with more physical meaning, i.e.

$$\begin{aligned}&\frac{\partial\mathscr{F}}{\partial t}+\frac{\partial V_i\mathscr{F}}{\partial x_i}-\frac{1}{\rho(\boldsymbol{\Psi})}\frac{\partial\langle p\rangle}{\partial x_i}\frac{\partial\mathscr{F}}{\partial V_i}+\frac{1}{\rho(\boldsymbol{\Psi})}\frac{\partial\langle\tau_{ij}\rangle}{\partial x_i}\frac{\partial\mathscr{F}}{\partial V_j}\\&\quad+\frac{\partial}{\partial\Psi_\alpha}\left[\frac{1}{\rho(\Psi)}\frac{\partial\langle J_i^\alpha\rangle}{\partial x_i}\mathscr{F}\right]+\frac{\partial}{\partial\Psi_\alpha}[S_\alpha(\Psi)\mathscr{F}]\\&\quad=\frac{1}{\rho(\boldsymbol{\Psi})}\frac{\partial}{\partial V_j}\left[\left\langle\frac{\partial p'}{\partial x_j}-\frac{\partial\tau'_{ij}}{\partial x_i}|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right]\\&\qquad-\frac{\partial}{\partial\Psi_\alpha}\left[\frac{1}{\rho(\Psi)}\left\langle\frac{\partial J_i'\alpha}{\partial x_i}|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right]\\&\qquad-\frac{\partial}{\partial\theta}\left[\left\langle\frac{\mathrm{D}\omega}{\mathrm{D}t}|\boldsymbol{V},\boldsymbol{\Psi},\theta\right\rangle\mathscr{F}\right].\end{aligned} \tag{3}$$

The variable J_i^α describes the scalar flux of scalar α in the x_i-direction, S_α is the chemical source term of scalar α and fluctuating quan-