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A multiple mapping conditioning mixing model with a mixture-fraction like reference variable. Part 1: Model derivation and ideal flow test cases

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ABSTRACT

Probability density function (PDF) methods have significant advantages in modeling turbulent combustion, in particular because the highly non-linear chemical source terms appear in closed form. The micromixing term in the PDF transport equations, representing diffusion in composition space, is however unclosed. Physically, micromixing occurs between regions of fluid having similar compositions. It is expected and generally shown that models that account for this localness of mixing perform better. In this work, a novel variation of the multiple mapping conditioning (MMC) mixing model is proposed. MMC makes use of reference variables to localise the mixing and was originally formulated for stochastic reference variables with standard Gaussian distributions. Here we follow the original interpretation but modify it by using a reference variable that has an evolving distribution, according to an Ornstein–Uhlenbeck process, with statistics that are similar to those of a physical scalar. In the present application of the model to nonpremixed combustion, mixture fraction is considered as the scalar; extensions of the model may be envisaged for other combustion modes by considering a different scalar variable. While the original version of MMC is mathematically elegant, it is conceptually complex and evaluation of model coefficients is difficult. The new model is both physically intuitive and its coefficients are easy to determine according to desired principles in canonical mixing situations. In Part I of this two-paper set, the model is studied analytically for homogeneous and mean scalar gradient flows without chemical reaction leading to an approach to set the model parameters that controls the unconditional scalar dissipation rate and delivers tunable localness. The behaviour of the model is also examined numerically in simple homogeneous mixing situations with and without chemical reaction. In Part II, the new MMC mixing model is implemented in the RANS context and validated against experimental data for the Sandia D–F flame series.

1. Introduction

Direct numerical simulation (DNS) of the instantaneous Navier–Stokes equations is computationally prohibitive for modeling practical combustion systems [1]. Reynolds-averaged Navier–Stokes (RANS) simulation or large-eddy simulation (LES) can reduce the computational cost by using averaging or filtering operations, respectively. The RANS expression for the evolution of the Favre averaged mass fraction, $\widetilde{Y_\alpha}$, of species, α, is

$$\frac{\partial \bar{\rho}\widetilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\widetilde{Y}_\alpha}{\partial x_i} + \frac{\partial \overline{J_i^\alpha}}{\partial x_i} = \overline{\omega_\alpha} - \frac{\partial \bar{\rho}\widetilde{u_i'Y_\alpha'}}{\partial x_i}, \tag{1}$$

where $\bar{\rho}$, $\tilde{u}_i$, $\overline{J_i^\alpha}$ are the mean density, Favre mean velocity and mean molecular flux of species, respectively. The averaging operation leads to the unclosed chemical source and turbulent scalar flux terms on the right-hand side (RHS) of Eq. (1) where the single prime denotes Favre fluctuations. The turbulent flux is commonly modelled with reasonable success using the gradient transport hypothesis [2]. On the other hand, the non-linearity of the chemical reaction rates and their interaction with the turbulent mixing makes modelling of $\overline{\omega_\alpha}$ difficult and various competing and complementary approaches have been suggested in the literature [2–4].

Turbulence–chemistry interactions (TCI) have a dominant effect on the formation of pollutants in practical combustors [5,6]. Conditional moment closure (CMC) [7], whereby the average reaction rate is approximated by integrating the conditionally averaged

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rate multiplied by the presumed PDF of the conditioning variable, has been a successful model for TCI. However, in practice it is usually limited to one particular mode of combustion and requires sometimes questionable models for the presumed PDF. It also becomes cumbersome when higher than first order conditional moments are required. Flamelet models [8] share some similarities with CMC but, unlike CMC, they are formally restricted to thin flame regimes. As a consequence of tabulation, flamelet models have advantages in terms of low computational effort. Composition PDF methods [9,10], which are much more general than CMC or flamelets, solve the transport equation for the one-point, one-time joint Eulerian PDF, f_ϕ, of the composition space, $\boldsymbol{\phi} = (\boldsymbol{Y}, h)$, where $\boldsymbol{Y} = (Y_1, \ldots, Y_\alpha, \ldots, Y_{n_s})$ is the vector of chemical species mass fractions and h is the mixture specific enthalpy. The transport equation for the Eulerian PDF is given by

$$\frac{\partial \rho f_\phi}{\partial t} + \frac{\partial \rho \tilde{u}_i f_\phi}{\partial x_i} + \frac{\partial \omega_k f_\phi}{\partial \psi_k} = -\frac{\partial}{\partial x_i}\left[\langle u_i'|\psi\rangle \rho f_\phi\right] + \frac{\partial}{\partial \psi_k}\left[\left\langle \frac{\partial J_i^k}{\partial x_i}|\psi \right\rangle f_\phi\right], \tag{2}$$

where ψ_k is the sample space variable for ϕ_k and the terms in angular brackets denote conditional Reynolds averages. In Eq. (2), ρ and ω_k are functions solely of ψ_k. Unlike many other combustion models, Eq. (2) does not in itself assume a particular combustion regime, and therefore the PDF approach can, in principle, be applied to all modes of combustion including non-premixed [11,12], premixed [13–17], stratified [18] and partially-premixed [19] modes. Additionally there is no assumption of thin reaction zones so that both fast and slow times scale processes, including those associated with pollutants [20], can be modelled. For these statements to be true in practice as well as in principle, the closures for the turbulent flux and conditional micro-mixing on the RHS of Eq. (2) must preserve the physically correct flame structure. As with the mean transport Eq. (1) a gradient model is commonly applied for the turbulent flux of the PDF. The conditional dissipation is modelled through a micromixing operation and, as discussed below, the available mixing models have limitations. Research into improving micromixing models is ongoing.

It is computationally efficient to recast Eq. (2) into an equivalent stochastic Lagrangian form and then solve for the evolution of notional particles [9]:

$$dx_i^* = \tilde{u}_i dt + \frac{1}{\bar{\rho}}\frac{\partial \Gamma_{eff}}{\partial x_i}dt + \sqrt{\frac{2\Gamma_{eff}}{\bar{\rho}}}dW_i, \tag{3}$$

$$d\phi_k^* = d\phi_{k,\omega}^* + d\phi_{k,mix}^* \,, \tag{4}$$

where the asterisk denotes particle properties, $W_i(t)$ is an independent isotropic Wiener process and Γ_{eff} is an effective diffusivity defined as

$$\Gamma_{\text{eff}} = \mu/\sigma + \mu_T/\sigma_T, \tag{5}$$

where μ and μ_T are the molecular and turbulent dynamic viscosities, respectively, and σ and σ_T are the molecular and turbulent Schmidt numbers. The terms $d\phi_{k,\omega}^*$ and $d\phi_{k,mix}^*$ represent the change in notional particle composition due to chemical reactions and mixing in composition space respectively, where the latter term is a model for the unclosed molecular mixing term in Eq. (2).

The simplest mixing model is interaction by exchange with mean (IEM), also known as linear mean square estimation (LSME) [21] written as

$$d\phi_{k,mix}^* = -\frac{1}{2}\frac{C_\phi}{\tau}(\phi_k^* - \widetilde{\phi_k})dt, \tag{6}$$

where $\widetilde{\phi_k}$ is the unconditional Favre mean obtained from the ensemble of particles at that location, τ is the turbulence time scale and C_ϕ is a model constant, nominally of order two. Subramaniam and Pope [22] nominate desirable characteristics of mixing models. IEM adheres to some of the important characteristics including conservation of means, decay of variances, boundedness, linearity with respect to scalar values and independence of mixing for each scalar. However, IEM violates the principles of localness, relaxation to a Gaussian PDF in homogeneous turbulence and ability to capture flamelet combustion. Other conventional models like Curl's [23] and modified Curl's [24] improve on IEM in that they can change the shape of the PDF but share the other drawbacks of IEM. The Euclidean minimum spanning tree (EMST) mixing model [22] is a higher quality model for most forms of combustion because it specifically introduces the localness property and performs well in flamelet conditions. However, EMST suffers some deficiencies as discussed in Ref. [25] including violation of linearity and independence and being prone to "stranding" in composition space and over-damping of conditional fluctuations [26]. Multiple mapping conditioning (MMC), derived by Klimenko and Pope [27], also introduces localness but does so using stationary Gaussian reference variables so that linearity and independence are satisfied and the scalars relax to Gaussian distributions in homogeneous turbulence. Other mixing models are under development including the parameterised scalar profile (PSP) model [28] and the shadow position mixing model (SPMM) [25]. The latter is an MMC-like model although the reference variables representing a shadow position of the notional particles have a different physical interpretation from the scalar reference variables normally used in MMC.

Vogiatzaki, Kronenburg and co-workers have developed the stochastic version of MMC-RANS in recent years [29–31]. They demonstrate how the dispersion between the reference variables, $\boldsymbol{\xi}$, having a stationary Guassian distribution, and the scalar fields, $\boldsymbol{\phi}$, can be used to independently model the conditional fluctuations while maintaining the correct rate of decay of the macroscale unconditional fluctuations. Deterministic implementations of original MMC are also available for both RANS [32] and LES [33] and these bear much resemblance to CMC. The mathematical elegance of original MMC implemented in this way is somewhat undermined by the complexity and non-linearity of the mapping functions which relate the Gaussian reference variables to the, in general, non-Gaussian scalar fields. MMC has evolved from its original form based on Markov-generated stationary Gaussian reference variables to a generalised model with other types of reference variables including those derived from a binomial Langevin model [34,35] and non-Markov Lagrangian quantities obtained from underlying DNS or LES fields [36].

In the present work, a novel, stochastic variant of the original formulation of MMC is developed. Rather than using a strictly Gaussian and stationary reference variable, the new reference variable is non-stationary and is designed to have similar statistics (namely mean and variance) to the mixture fraction. The model retains the inherent strengths of MMC in satisfying many of the characteristics of a quality mixing model and additionally has the advantage of being physically more intuitive than the original formulation. As a consequence the model coefficients are more easily determined and the numerical implementation is robust.

The governing equations and properties of the new MMC mixing model are described in Section 2. In Section 3, the mixing model is analysed in the context of homogeneous, isotropic, inert, turbulent flow. A statistically stationary case with a mean scalar gradient is also considered. An approach to setting the model coefficients that provides a physically specifiable dissipation rate for unconditional scalar fluctuations and an independently specifiable degree of localness is outlined based on analytical results for these two cases. The model behaviour is also studied numerically in the homogeneous test case. The model performance for the homogeneous flamelet combustion test case of Norris and Pope [37] is investigated in Section 4. The controlled enforcement of mix-