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A DNS Evaluation of a Novel Multiple Mapping Conditioning Model with a Mixture Fraction-like Reference Variable

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Abstract

One of the main challenges of the transported probability density function (TPDF) method for reactive flow simulation is to accurately model the unclosed molecular mixing term. Recently, a novel, conceptually simplified, Multiple Mapping Conditioning (MMC) mixing model with a mixture fraction-like reference variable (hereafter referred to as SMMC model) was proposed for simulating nonpremixed turbulent flames. In this model, a reference variable is designed to be statistically similar to mixture fraction. Scalar mixing occurs in two levels: major mixing by evolvement of a reference variable and minor mixing of scalars toward their mean conditional on the reference variable. A target correlation coefficient between the reference variable and mixture fraction, r_t, is introduced to change the localness of the model. In the original SMMC model, coefficients are derived for a spatially zero-dimensional, homogeneous isotropic turbulence (HIT) reference case at statistically steady state. In the present work, we extend this method by considering a spatially one-dimensional, homogeneous flow with a uniform mean scalar gradient (MSG). With this new configuration, the coefficients of the two-level scalar mixing operators can be determined by r_t. Three DNS datasets with strong extinction-reignition events are used for comparison as well as to provide the input data for the TPDF simulations. The results with coefficients determined from the MSG configuration (SMMC-MSG) are compared to that determined from the HIT case (SMMC-HIT). Both sets of model coefficients give good predictions of mean mixture fraction and temperature for properly chosen r_t values, with little difference observed between the two models with respect to the mean values. It is also found that the coefficients obtained from the SMMC-MSG case correctly predict the mixture fraction variances over a wide range or r_t values, while the coefficients from the SMMC-HIT case only yields correct predictions when r_t is large, corresponding to the situation with high localness.

Introduction

The transported probability density function (TPDF) method provides a computationally tractable approach to modelling turbulent reactive flows [2, 6]. The general idea of the TPDF method is to devise a system of notional particles whose evolution yields the same one-point, one-time Eulerian PDF as the real fluid particle system. This method has the important advantage that the nonlinear chemical source term appears in closed form, whereas the challenge is the modelling of the unclosed molecular mixing term. Various molecular mixing models have been proposed within the TPDF framework, e.g., the Interaction by Exchange with the Mean (IEM) model [12] and the Euclidean Minimum Spanning Tree (EMST) model [8]. Subramaniam and Pope [8] have proposed desirable properties of a mixing model to guide their development and evaluation. For example, a mixing model should satisfy the principle of localness (mixing takes place locally in composition space) and independence (mixing of one scalar should not be influenced by others). None of the existing models possesses all the desirable properties, although some models satisfy several of the most important criteria, e.g., the EMST model ensures the localness of mixing at the cost of independent mixing. Mixing models developed within the Multiple Mapping Conditioning (MMC) framework [3] posses in principle the ability to control the localness of mixing without formal violation of the principle of independence.

Recently, a novel, conceptually simplified, MMC model was proposed [10, 9] (hereafter referred to as SMMC model). The SMMC model is a novel variant of the original formulation of the MMC model. 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) as the real mixture fraction. The model retains the inherent strength of the MMC method and thus satisfies many of the desirable properties for a mixing model and additionally has the advantage of being physically more intuitive and easier to implement.

In the original work [10], the coefficients of the SMMC model were specified to yield a correct solution of the scalar variance decay in a homogeneous isotropic turbulence (HIT) reference case. It was demonstrated numerically that this coefficient set (SMMC-HIT) works well in a reactive jet flow with strong localised extinction [9], and diesel spray combustion [11] for coefficients that lead to a highly local mixing model. However, it is unknown whether this set of model coefficient works for other flow configurations with more complexities, e.g., reactive mixing layers with near-global extinction and reignition with a bimodal PDF, as exhibited by a recent DNS study [5]. Aside from a more extensive evaluation of the SMMC model with the originally proposed coefficient set, an alternative set of model coefficients based on a reference case with homogeneous turbulence and a uniform mean scalar gradient (MSG) has been proposed [10] (hereafter referred to as SMMC-MSG). This alternative set of model coefficients has not yet been evaluated in combustion simulations.

The objectives of the current study thus are: (1) to evaluate the SMMC mixing model with the HIT coefficient set for modelling a series of Direct Numerical Simulation (DNS) of nonpremixed turbulent flames with increasing extinction-reignition events and (2) to assess and compare the performance of the model with the alternative MSG coefficient set for these flames.

The remainder of the paper is structured as follows: first the governing equations of the SMMC model and its coefficient settings are presented; second the numerical methods for solving the equations and the configuration of the DNS are introduced; finally the results of both the SMMC-HIT and SMMC-MSG models are presented, with a comparison against DNS results.

Model description

In the current study, we adopted the composition transported probability density function approach [2, 6], in which the joint PDF of chemical species and an energy variable (enthalpy in the current study) is evolved. Due to the multidimensionality of the sample space, the transport equation for the joint composition PDF is solved in a stochastic way with a system of Lagrangian particles which aims to yield a consistent Eulerian PDF of the real flow field. The governing equations for the particles are:

$$dx^* = [\tilde{u} + \frac{\nabla\overline{\rho}\widetilde{\Gamma}}{\overline{\rho}}]dt + \sqrt{2\tilde{\Gamma}}dW, \tag{1}$$

$$d\phi^* = d\phi^*_{mix} + d\phi^*_{react}. \tag{2}$$

In the above equations, the Favre-average of ψ, denoted as $\widetilde{\psi}$, is defined as $\widetilde{\psi} = \overline{\rho\psi}/\overline{\rho}$, where ρ is the density and the overbar represents a Reynolds-averaged quantity. Equation (1) represents the transport of particles in physical space, which is comprised of a deterministic part, $[\tilde{u} + \nabla\overline{\rho}\widetilde{\Gamma}/\overline{\rho}]dt$ and a stochastic part, $\sqrt{2\widetilde{\Gamma}}dW$. The deterministic part represents the effects of the mean velocity field $\tilde{u}$ and the turbulent diffusion, which is modelled using the gradient diffusion hypothesis. The stochastic part is a Wiener process that models the turbulent transport as a random walk with step-size proportional to the square root of the turbulent diffusivity $\widetilde{\Gamma}$. In the current study, both the mean velocity $\tilde{u}$ and the turbulent diffusivity $\tilde{\Gamma}$ are inputs from the DNS data with $\tilde{\Gamma}$ calculated as $\tilde{\Gamma} = -(\widetilde{\rho u Z} - \overline{\rho}\tilde{u}\tilde{Z})/\overline{\rho}\nabla\tilde{Z}$, where Z is the mixture fraction.

Equation (2) represents the particle transport in composition space. The key part for modelling is the first term in equation (2), $d\phi^*_{mix}$, which represents the micro-mixing process of the composition scalars. In the SMMC model, scalar mixing occurs in two levels: (i) the major mixing of the reference variable, ξ, which evolves by an Ornstein–Uhlenbeck (OU) process (equation 3) and (ii) the minor mixing of the scalars, ϕ, by relaxation towards their mean conditional on ξ (equation 4).

$$d\xi^* = -\frac{C_\xi}{\tau}(\xi^* - \widetilde{\xi})dt + b_0\sqrt{\frac{2C_\xi\widetilde{\xi'^2}}{\tau}}dW_\xi, \tag{3}$$

$$d\phi^*_{mix} = -\frac{C_{min}}{\tau}(\phi^* - \widetilde{\phi|\xi})dt. \tag{4}$$

The three model coefficients, C_ξ, C_{min}, b_0 need to be specified consistently to obtain the desired model properties, i.e. statistically similar reference variable, ξ, and mixture fraction, Z [10]. To achieve this, a correlation coefficient, r, between ξ and Z is introduced:

$$r = \frac{\widetilde{\xi'Z'}}{\sqrt{\widetilde{\xi'^2}\widetilde{Z'^2}}}. \tag{5}$$

The specification of the SMMC model coefficients is then based on the following two principles:

1. The implied unconditional scalar dissipation rate is consistent with the model $d\widetilde{\phi'^2}/dt = -C_\phi\widetilde{\phi'^2}/\tau$.

2. The correlation coefficient r approaches a target value, r_t.

The settings to achieve these outcomes are flow dependent. The method here to obtain the model coefficients is similar to that in [10, 9]. Briefly speaking, the analytical solution for the scalar variance $\widetilde{\phi'^2}$ is equated to the imposed scalar variance decay in the model (principle 1), and the analytical solution of r at steady state is equated to a user-specified target value, r_t (principle 2). In this way, the coefficients of the SMMC model can be expressed as a function of r_t. Table 1 summarises the coefficient sets based on the HIT and MSG reference cases. It should be noted that the two sets of model coefficients approach each other when r_t approaches unity.

	SMMC-HIT	SMMC-MSG
C_{min}	$\frac{C_\phi}{2(1-r_t^2)}$	$\frac{C_\phi}{2(1-r_t^2)}$
C_ξ	C_ϕ	C_ϕ/r_t
b_0	$\sqrt{1/2}$	$\sqrt{1-r_t/2}$

Table 1: Coefficient settings for SMMC model

In an a-posterior RANS simulation, the turbulent mixing frequency Ω is commonly modelled as $\Omega = C_\phi/\tau$, where C_ϕ is a free parameter of order unity and the turbulent time scale, τ, is modelled as the ratio of turbulent kinetic energy to turbulent dissipation rate. Here, the turbulent mixing frequency Ω is also provided by the DNS similar to u and Γ, and calculated as the ratio of Favre-averaged mixture fraction variance to Favre-averaged scalar dissipation rate.

Numerical Methodology

A symmetric splitting scheme is used to solve equations (1)–(4). Each time step is divided into substeps in which the individual process of transport, mixing and reaction occurs sequentially. This scheme is denoted as **TMRMT** [13], in which **T** stands for transport in physical space, **M** for mixing of ξ and ϕ, and **R** for chemical reactions.

The conditional mean $\langle\phi|\xi\rangle$ in equation (4) is implemented in a similar way as in [10]. Particles in each mesh cell are first sorted in ascending order in ξ space. The conditional mean of the j-th sorted particle $\langle\phi^j|\xi\rangle$, is approximated by the mean of its two nearest neighbour particles in ξ space, that is:

$$\langle\phi^j|\xi\rangle = \frac{1}{2}(\phi^{j+1} + \phi^{j-1}). \tag{6}$$

For the particles at the boundaries, i.e., the particles with the minimum and maximum ξ values in each cell, the conditional mean is approximated by the mean of its inner neighbour and itself, that is:

$$\langle\phi^1|\xi\rangle = \frac{1}{2}(\phi^1 + \phi^2),\ \langle\phi^n|\xi\rangle = \frac{1}{2}(\phi^n + \phi^{n-1}). \tag{7}$$

where n is the number of particles in each cell. The number of particles per cell is 200.

DNS and simulation scenario

Three DNS datasets of turbulent nonpremixed ethylene flames [5] with increasing extinction levels (Case 1, 2, 3) are used for comparison. The three-dimensional DNS data are statistically one-dimensional and allow for spatial averaging in both the streamwise and spanwise directions. Hence the comparison between the SMMC model and the DNS dataset is performed along the one-dimensional cross-stream direction, y, normalized by the characteristic height, H. The evaluation follows the approach in our previous study [4]. Only the results for Case 1 at 60 jet times are presented for brevity. The conclusion drawn

from the results of Case 2 and 3 are similar to that of Case 1 with respect to the analysis in the current study.

Results and discussions

Mixture fraction mean and variance

Figure 1 shows the mean mixture fraction profile at 60 jet times with different r_t values. The mean profile of mixture fraction,

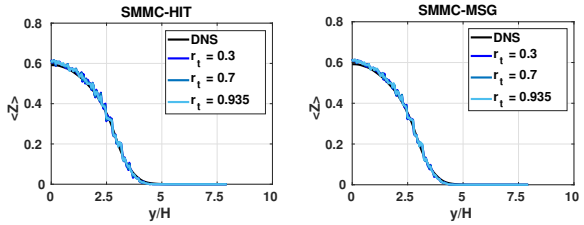

Figure 1: Mean profile of mixture fraction $\widetilde{Z}$ with different target r_t values at 60 jet times by the SMMC-HIT (left) and SMMC-MSG (right) models

$\tilde{Z}$, is well predicted by both the SMMC-HIT and SMMC-MSG models. This is expected since by construction the turbulent flow information are extracted from the DNS. There is little difference between SMMC-HIT and SMMC-MSG in terms of $\tilde{Z}$ since the mixing process does not affect the mean of mixture fraction either directly or indirectly through the coupling with chemical reactions [4]. The correct prediction of the mixture fraction provides confidence that the numerical implementation of the particle method is correct.

Figure 2 shows the mixture fraction RMS, Z_{rms}, profiles at 60 jet times with different r_t values. It is found that the SMMC-MSG

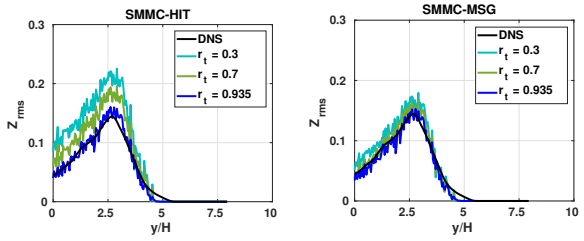

Figure 2: Profile of Z_{rms} with different target r_t values at 60 jet times by SMMC-HIT (left) and SMMC-MSG (right) models

model yields a good agreement for Z_{rms} over a wide range of r_t values, while the SMMC-HIT model only yields a good agreement when r_t approaches unity, i.e., when ξ and Z are highly correlated, leading to a high level of localness in the SMMC mixing model. Therefore, setting the SMMC coefficients according to the MSG case allows the localness of the model to be varied without adversely affecting the prediction of Z_{rms}, in contrast to the HIT settings which results in an over-prediction of Z_{rms} for less local models.

Mean profile of temperature

Figure 3 shows the profile of mean temperature at 60 jet times with different r_t values. It is found that both the SMMC-HIT and SMMC-MSG model yield good predictions for the mean temperature with the default value for the correlation coefficient, r_t=0.935 [10]. It also shows that decreasing r_t leads to increasing levels of extinction. This is because decreasing r_t leads to a lower correlation between ξ and Z, and thus mixing is less local in composition space (here approximated by mixture

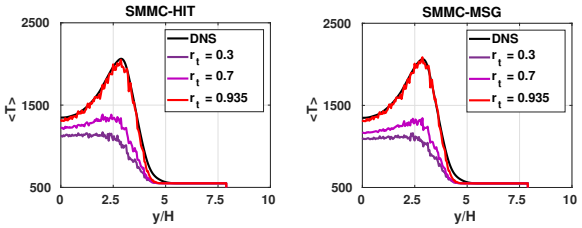

Figure 3: Mean profile of temperature T with different target r_t values at 60 jet times by SMMC-HIT (left) and SMMC-MSG (right) models

fraction-like reference space). For the current ethylene flame, which is mainly composed of thin nonpremixed flamelets [5], less localness will make the mixing process directly jump over the reaction zone and increase the the degree of extinction. This supports the notion that localness in composition space is an important consideration for developing TPDF mixing models.

Conditional PDF

Figure 4 shows the conditional PDF of mixture fraction at 60 jet times by the SMMC-HIT and SMMC-MSG models with different r_t values. It is found that the performance of SMMC-HIT and SMMC-MSG are similar. When r_t is small (e.g. $r_t = 0.3$), the flame extinguishes and the temperature of individual particles fluctuates mainly around the extinction branch. Increasing r_t makes more particles transit to the ignition branch (e.g. $r_t = 0.7$) although the flame is still globally extinguished (see also Fig. 3). When r_t further increases (e.g., $r_t = 0.935$), the mixing model becomes highly local and the flame is fully ignited. It is also found that increasing r_t leads to a narrower PDF width. For comparison, the results of the IEM model and the EMST model are also presented. It is shown that the IEM model wrongly picks the extinction branch and the EMST model predicts the ignition branch with an over-narrowed PDF. For the SMMC model, small r_t can reproduce results similar to the IEM model and larger r_t similar to the EMST model.

Conclusions

In this work, we parameterise the SMMC model with two different coefficient sets obtained from homogeneous isotropic turbulence (HIT) and homogeneous turbulence with a mean scalar gradient (MSG) reference cases, and evaluate the model performance against a DNS turbulent nonpremixed flame with strong extinction-reignition events. The main findings include:

- Both SMMC-HIT and SMMC-MSG yield good prediction for mean temperature when the mixing is highly local.
- SMMC-MSG yields better results for mixture fraction variance than SMMC-HIT over a wide range of r_t value.
- r_t can be used to change the localness of SMMC model.
- Further work includes applying the current method for the SMMC model coefficient specification using a correlation coefficient to other MMC-type models such as the Shadow-Position Mapping Mixing (SPMM) model [7].

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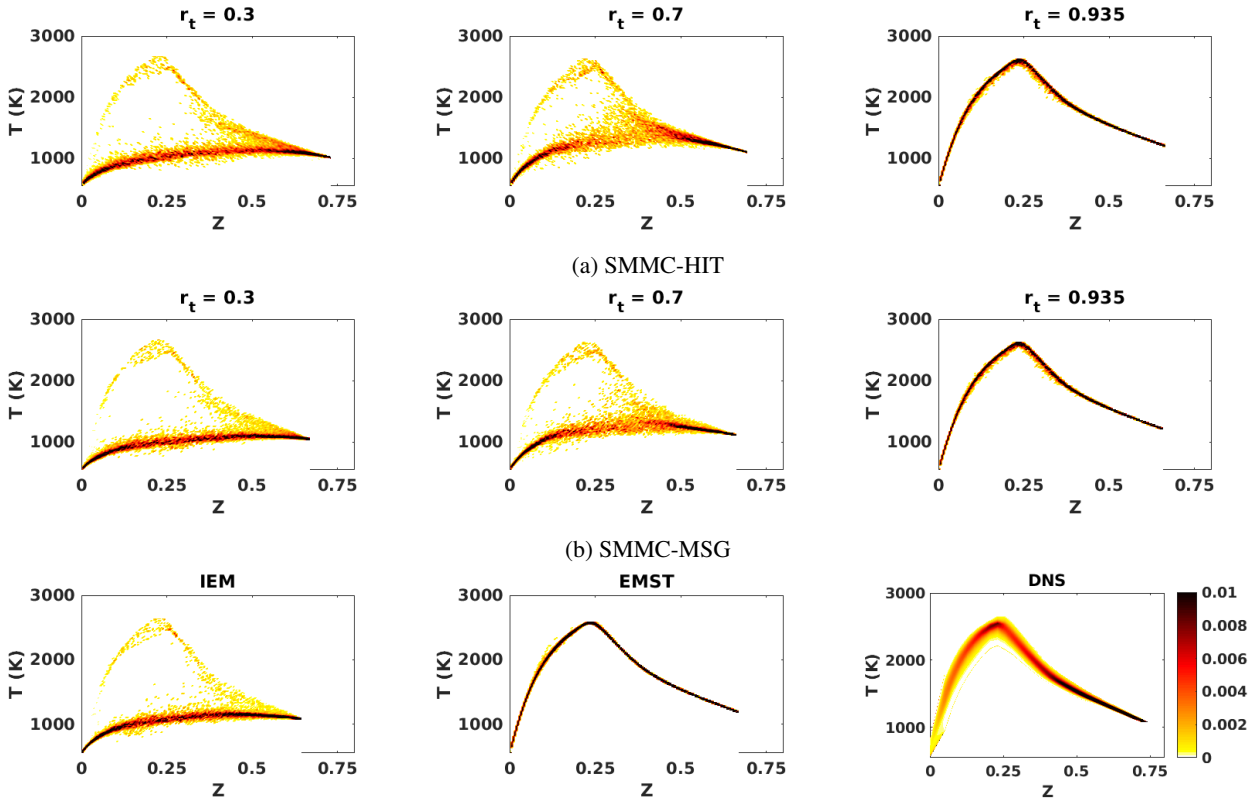

(a) SMMC-HIT

(b) SMMC-MSG

(c) IEM, EMST, DNS

Figure 4: PDF of temperature conditional on mixture fraction at 60 jet times for Case 1. First row: SMMC-HIT model with different r_t values; second row: SMMC-MSG model with different r_t values; third row: IEM, EMST and DNS models.

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