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Evaluating the Shadow Position Mixing Model for Transported PDF Modelling of Non-Premixed Flames

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Abstract

Mixing models, which account for the effect of molecular diffusion on the composition field, remain an area of uncertainty when using the Transported Probability Density Function (TPDF) Method. A recently proposed mixing model, the Shadow Position Mixing Model (SPMM), attempts to provide a physically valid mixing model for use in TPDF methods. The SPMM models the mixing process is as a relaxation of the composition to the mean composition conditioned on a new variable, the shadow position. This study compares the performance of the SPMM against the Interaction by Exchange with the Mean (IEM), Modified Curls (MC) and Euclidean Minimum Spanning Tree Model (EMST) models as well as reactive Direct Numerical Simulation (DNS) data. The SPMM implementation was validated against a non-reacting, uniform scalar gradient interacting with homogeneous isotropic turbulence. The reacting test case was a one-dimensional, nonpremixed, turbulent jet flame burning a syngas fuel stream which exhibited strong extinction and reignition events. DNS data was used to provide input data to the TPDF simulations in order to remove the uncertainty surrounding the modelling of the turbulence. It is found that the SPMM was able to accurately capture the extinction and reignition events and could produce mean temperature and mixture fraction profiles which compared well to the DNS. The agreement for conditional temperature PDFs were dependent on the model constants chosen. The results could be adjusted to be similar to IEM or EMST for different choices of model constants.

Introduction

Transported Probability Density Function (TPDF) methods [6, 7] are an effective means of modelling turbulent combustion systems. While other methods solve for low order moments or conditional moments, the TPDF method solves for the whole one point PDF of composition (or velocity and composition) by solving evolution equations for point samples of the fluid. This results in the chemical source term appearing in closed form.

While the chemical source term is closed in the TPDF formulation, a mixing model is required to close the molecular diffusion term [1, 5]. These mixing models represent an area of uncertainty for TPDF methods. The three most commonly used mixing models are: the Interaction by Exchange with the Mean (IEM) [10], the Modified Curl's (MC) [2], and the Euclidean Minimum Spanning Tree (EMST) [9] models. These three models all have limitations in terms of their applicability or physical validity despite their widespread use. For example, the EMST model tends to produce PDF's with artificially small conditional fluctuations while the IEM model does not represent the physical process of mixing well as it cannot account for the stochastic nature of turbulence [4].

A new mixing model, the Shadow Position Mixing Model (SPMM), was proposed by Pope [8] to address the shortcomings of these models. The SPMM models the mixing interactions between these notional particles as a relaxation of the composition to the mean composition conditioned on a new variable, the shadow position (Z). This study will evaluate the SPMM by comparing it against the aforementioned mixing models with respect to their performance in modelling a Direct Numerical Simulation (DNS).

The remainder of the paper is structured as follows. Firstly, the methodology and governing equations are presented. This is followed by a description of the verification and validation used to test the SPMM implementation. Finally the results for the reacting DNS case are presented.

Modelled Transport Equations

The TPDF model is based on a Reynolds-Averaged Navier Stokes (RANS) formulation where the turbulence closure is provided directly from the DNS data. Stochastic differential equations, describing the evolution of the particle location (equation 1) and composition (equation 2) are solved for each particle. For the SPMM an additional equation (equation 3) describing the evolution of the particle shadow position is solved. The stochastic equations are given as:

$$d\mathbf{X}(t) = [\tilde{V} + \frac{\nabla\tilde{\Gamma}_T\bar{\rho}}{\bar{\rho}}]dt + \sqrt{2\tilde{\Gamma}_T}d\mathbf{W} \tag{1}$$

$$d\phi(t) = [\mathbf{M}]dt + \mathbf{R}dt \tag{2}$$

$$d\mathbf{Z}(t) = \tilde{V}dt - \bar{a}\Omega_\phi(\mathbf{Z}-\mathbf{X}) + \bar{b}\sqrt{2\tilde{\Gamma}_T}d\mathbf{W}' \tag{3}$$

In equation 1 and 3, $\tilde{V}$ is the mean velocity field, Γ_T is the turbulent diffusion coefficient. Γ_T is defined as $\Gamma_T = -\left(\frac{\widetilde{\rho V\xi} - \bar{\rho}\tilde{V}\tilde{\xi}}{\bar{\rho}\nabla\tilde{\xi}}\right)$, where ξ is the mixture fraction. In equation 2, $[\mathbf{M}]$ and $\mathbf{R}$ represent the change in particle composition due to mixing and chemical reaction, respectively. In equation 3, Z is the shadow position, Ω_ϕ is the mixing frequency which is defined as $\Omega_\phi = \frac{\widetilde{\chi_\phi}}{\widetilde{\xi''^2}}$, where $\widetilde{\chi_\phi}$ and $\widetilde{\xi''^2}$ are the Favre averaged scalar dissipation and Favre averaged mixture fraction variance, respectively. The scalar dissipation is defined as, $2\widetilde{D|\nabla\xi|^2}$ where D is the mass

diffusivity of N_2. The random fluctuations produced by turbulence are modelled by the independent Wiener processes, $d\mathbf{W}'$ and $d\mathbf{W}$ [11]. equation 3 has two model coefficients, $\overline{a}$ and $\overline{b}$, which need to be set a priori.

A symmetric splitting scheme is used to solve equations 1-3. Each time step is subdivided into partial steps in which the individual processes of transport of position and shadow position, mixing and reaction occur individually. This scheme is denoted as **TSMRMST** [11, 12], where each letter represents an individual process. **T** represents transport of the position in physical space, **S** represents transport of the shadow position in physical space, **M**, molecular mixing and **R**, chemical reaction.

The mixing step is evaluated using a formulation similar to the IEM model. However, instead of mixing based on the mean conditional on particle position an additional conditioning variable, the shadow position, is used. This leads to the model:

$$\frac{d\phi}{dt} = \overline{c}\Omega_\phi(\phi - \langle\phi|\mathbf{Z},\mathbf{X}\rangle) \tag{4}$$

where $\overline{c}$ is a model coefficient. This model is a relaxation to the mean composition conditional on the shadow position. The combination of $\overline{a}$, $\overline{b}$ and $\overline{c}$ determines the evolution of the shadow position and the combination of coefficients determines how local the SPMM mixing process is.

To evaluate the conditional mean, $\langle\phi|\mathbf{Z},\mathbf{X}\rangle$, in equation 4 the approach taken by Pope [8] is adopted. For the n^{th} particle, the conditional mean is approximated as:

$$\langle\phi|\mathbf{Z}^n,\mathbf{X}^n\rangle = \frac{1}{2}[\phi^{n+1} + \phi^{n-1}] \tag{5}$$

The particle n has it's composition updated by the average composition of it's two nearest neighbours in shadow position space. For the end points, the opposite end point is used as a nearest neighbour. For example, the n=1 particle has nearest neighbours n=2 and n=n.

Verification

The SPMM was implemented in a TPDF code that has been used previously to test the IEM, MC and EMST models for non-premixed combustion [4]. To verify the implementation of the new model, a non-reacting Mean Scalar Gradient (MSG) case was set up modelling turbulent diffusion and mixing of a passive scalar with a uniform mean gradient. The MSG case was chosen as analytical results are available. The case had the following parameters. The domain was one dimensional from -0.1 m to +0.1 m, $\Gamma_T = 1\times10^{-4}m^2/s$, $\Omega_\phi = 1s^{-1}$, the velocity field was set to zero everywhere. The scalar of interest (ϕ) was initially set as $\phi = G\times y$, where G is the scalar gradient which takes value 100 m^{-1}. A jump periodic boundary condition was applied on the scalar to preserve the mean gradient indefinitely. The fluctuation of the scalar (ϕ') in the mean scalar gradient case evolves by the following:

$$d\phi' = -\overline{c}\Omega_\phi(\phi' - \langle\phi'|\mathbf{Z}\rangle)dt - G(2\Gamma_T)^{1/2}d\mathbf{W} \tag{6}$$

In the mean scalar gradient case the normalised variance of the mixture fraction field (V_ϕ) is analytically given by:

$$V_\phi = \frac{1}{\overline{c}} + \frac{1}{q} \tag{7}$$

where $q = \frac{\overline{a}(1+\overline{b}^2)}{4\overline{c}}$. This is the statistically stationary solution for the second moment of the scalar evolution equation [8].

To test the implementation of the SPMM, various values of V_ϕ and q were selected. Values for $\overline{a}$, $\overline{b}$ and $\overline{c}$ can then be determined from equation 7. If the implementation is correct then the normalised scalar variance from the simulation should match the scalar variance calculated from the model coefficients. A range of V_ϕ values were tested and q took values 0.1, 0.5, 1.0 and 1.5. The value for $\overline{b}$ was set to either 1 or 0 for simplicity. The choice to only use two values of $\overline{b}$ is justified as the only condition that needs to be satisfied is:

$$\overline{a}(1+\overline{b}^2) = 4\overline{c}q \tag{8}$$

Thus, the specification of $\overline{a}$ and $\overline{b}$ is immaterial [8] and so only two simple specifications for $\overline{b}$ are tested.

All cases were run with 96 cells and 1000 particles per cell. Fig. 1 shows that the output variance is approximately equal to the analytical V_ϕ value for all values of q, evident from each line having approximately unity gradient. The variation from unity is likely due to the statistical error.

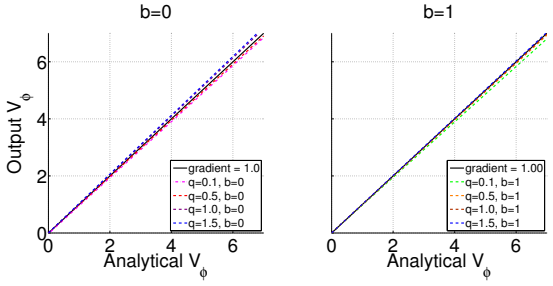

Figure 1. Mean Scalar Gradient case, comparison of analytical and simulated solutions for coefficient $\overline{b} = 0$ (left) and $\overline{b} = 1$ (right).

Simulation Scenario

The DNS simulated a temporally evolving, turbulent planar-jet flame. The full details of the simulations are given in [3], and only a brief summary will be given here. The DNS was initialised with a three-dimensional planar slab of syngas fuel (CO and H_2) in counter flow with oxidiser streams on either side. A small turbulent velocity fluctuation was imposed at the initial time which generated the instabilities in the shear layer between the fuel and oxidant streams. The Reynolds number (Re) was parametrically varied, where Re took values 2510, 4478 and 9079. This study will only consider the middle, $Re = 4478$ case. This configuration is statistically one dimensional, and allows for ensemble averaging in both the streamwise and spanwise directions, leaving a statistical dependence on the transverse direction, $\hat{y}$, and the time, t. The ensemble average is performed on a mass (Favre) basis. This DNS was chosen as it featured strong extinction and re-ignition events, which are difficult to capture in RANS simulations and show strong sensitivity to the mixing model.

Results

Mean and RMS profiles

The mean mixture fraction profiles (figure 2) provide verification that the physical transport models have been implemented correctly. The SPMM model performs comparably with the other models for the syngas test case, producing equivalent results. This is expected, as the mixing process does not affect the mean mixture fraction profile and gives assurance that the physical transport models for the particles is correct.

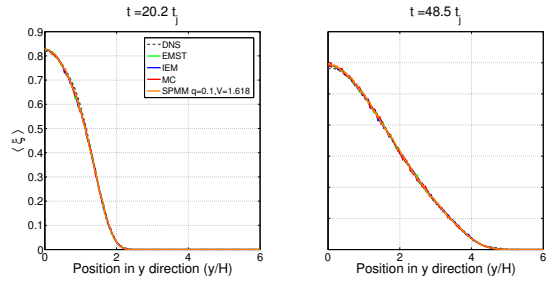

Figure 2. Comparison of mean mixture fraction profiles for each mixing model at 20 jet times (left) and 48.5 jet times (right)

The mixture fraction RMS profile can be used to determine if the mixing process is occurring at the correct rate. The mixture fraction RMS profiles for the IEM, MC and EMST models are all very similar. This is because the scalar dissipation rate is known completely for these three models. At both times these models overpredict the mixture fraction RMS. The dissipation rate for the SPMM depends on the $Z-\phi$ correlation and so is not known. Thus, the coefficients for the SPMM were fitted to produce a mixture fraction RMS profile which matched the DNS.

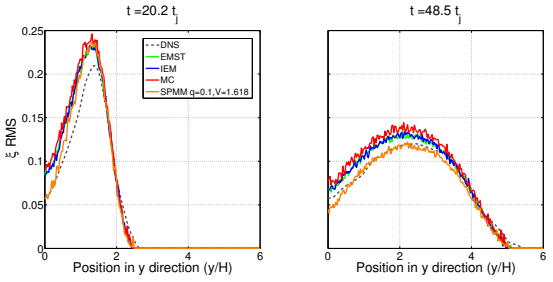

Figure 3. Comparison of mixture fraction variance profiles for each mixing model at 20 jet times (left) and 48.5 jet times (right)

The temperature characterises the thermochemical state of the system, thus it can be used to study the effect of mixing on other process such as chemical reaction. When considering the mean temperature profiles, the SPMM performs better than the EMST model with particular choices of model constants as demonstrated by figure 4. In this study, the EMST model outperforms the IEM or MC models however, the EMST model over predicts the spatial profile of the temperature at the latter times. The SPMM matches the DNS closely using the model coefficients determined by matching the DNS mixture fraction RMS. This is consistent with the study by Krisman et al. [4]. The EMST model, the most local in composition space, performed significantly better than the IEM or MC models when considering the mean temperature profiles. The EMST model was the only model to correctly reproduce the extinction characteristics in the ethylene flame. In this study the two local models in composition space (EMST and SPMM) perform significantly better than the models which are non-local (IEM and MC). This supports the idea that locality in composition space is an important constraint to consider in the development of mixing models.

Conditional Temperature

Figure 5 and figure 6 show the effect of varying the parameter q on the PDF of temperature conditional on mixture fraction. The SPMM produces behaviour similar to both the EMST and IEM. For large values of q, that is, tending towards completely non-local mixing, the SPMM behaves similarly to the

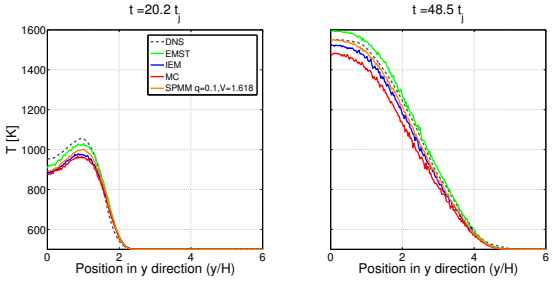

Figure 4. Comparison of mean temperature profiles for each mixing model at 20 jet times (left) and 48.5 jet times (right)

IEM model. The PDF is much broader than the EMST and similar in shape to both the DNS and IEM model. This indicates significant conditional fluctuations in temperature. It is expected if q were equal to infinity the IEM and SPMM predictions would be identical. As q tends towards zero the SPMM becomes a more local model, appearing similar to the EMST model. The PDF becomes very thin, showing small conditional fluctuations. This a result of the localness of the mixing process, the EMST model is a highly local mixing model that only mixes the particles close together in composition space. Similarly, by setting the value of q close to zero the mixing becomes highly local both in physical and composition space. Thus a similar behaviour is observed when comparing the EMST and the SPMM. This is consistent with Krisman et al. [4] as the models which are highly local in composition space produce narrow PDFs.

From the results presented above, the SPMM has demonstrated its potential as a more general and flexible description of mixing as well as improved model prediction of turbulent reactive flow.

Conclusion

The Shadow Position Mixing Model (SPMM) has been implemented and validated in the context of a RANS, C-TPDF simulation. The performance of this model was compared to the IEM, MC and EMST models. Mean velocity, turbulent diffusivity and mixing frequency fields were used as inputs to allow for direct comparisons between each model by reducing the number of model assumptions in the simulation. The SPMM was capable of producing results comparable to the EMST model in terms of mean temperature and mixture fraction profiles and extinction and re-ignition characteristics. The SPMM was also seen as the most flexible model capable of producing behaviour similar to the EMST or IEM depending on how the model coefficients were chosen.

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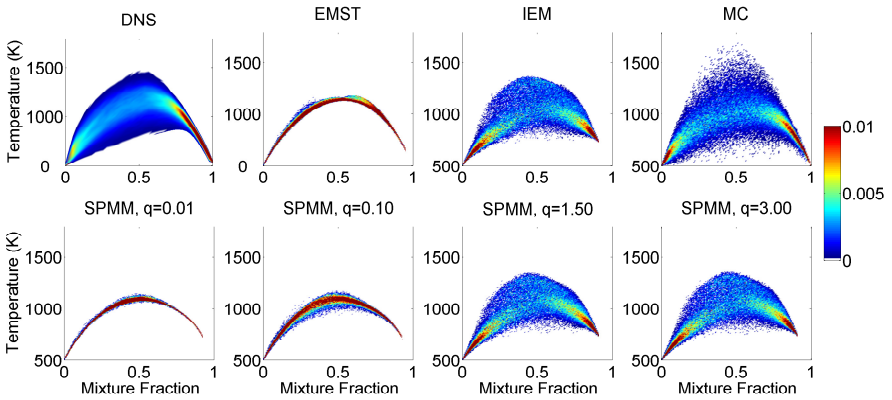

Figure 5. Comparison of temperature conditional on mixture fraction for at 20 jet times. The top row of plots represents the three original models and the DNS. The bottom row of plots is the SPMM using different values of q.

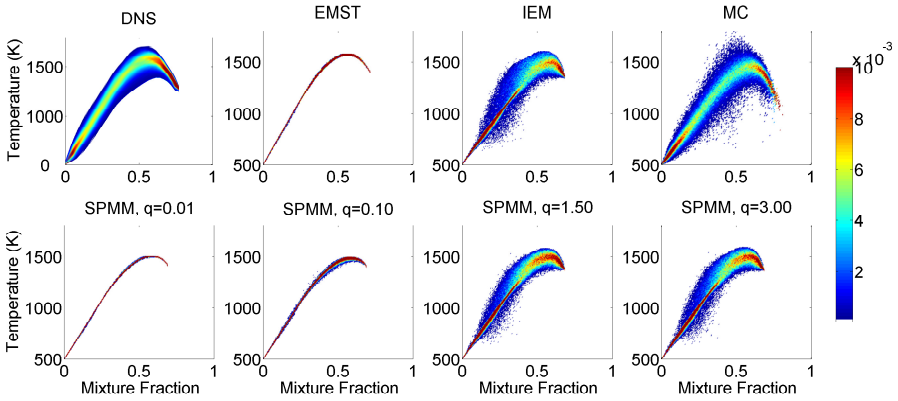

Figure 6. Comparison of temperature conditional on mixture fraction for at 48.5 jet times. The top row of plots represents the three original models and the DNS. The bottom row of plots is the SPMM using different values of q.

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