A DNS evaluation of the effect of mixing models on soot predictions in nonpremixed ethylene flames using the transported PDF method

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Abstract

Soot presents a significant challenge to mixing models in the transported probability density function (TPDF) method, owing to its vastly larger Schmidt number compared with gas-phase species. The objective of the present work is to provide guidance for selection of mixing models for soot in TPDF frameworks by comparison of model outcomes to direct numerical simulation (DNS) results. DNS of a sooting, nonpremixed, turbulent jet flame with ethylene fuel is used. For the TPDF model, the study examines three of the most widely used mixing models: interaction by exchange with the mean (IEM), modified Curl (MC) and Euclidean minimum spanning tree (EMST). Two extremes of soot mixing treatment are considered, one in which soot is not mixed, and one in which it is mixed at the same rate as the gas-phase species. To limit possible sources of error to the mixing model, the DNS was used to provide key inputs over the course of the runs, including the mean flow velocities, mixing frequency, and the turbulent diffusion coefficient. It is found that the TPDF method is successful at predicting the temperature profiles and, with no soot mixing, the soot mass fraction profiles, when using EMST for the gas phase. In contrast, the IEM and MC models overpredict the amount of extinction compared to the DNS and therefore do not predict the soot production accurately. Concerning soot mixing, it is found in conjunction with EMST that no soot mixing produces superior results to mixing soot at the same rate as gas-phase species. However, an overprediction of the root-mean-square (RMS) soot mass fraction is observed. In contrast, the mean and RMS soot mass fractions are underpredicted when soot mixing was considered. This may imply that the effective mixing rate of soot is non-zero but not as high as the gas-phase mixing rate.

Keywords:

TPDF methods, DNS, soot, mixing models

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1. Introduction

The harmful effects of soot on health and the environment motivate the development of predictive models for soot emission. Soot presents difficult modelling challenges owing to the complexity of the gaseous precursor chemistry, the processes of inception, surface growth, agglomeration and oxidation, and high levels of intermittency [1]. Also important is that timescales of processes involved in soot formation are often much longer than typical combustion timescales, creating difficulties for the application of scale-separation assumptions often applied in fast chemistry models of turbulent combustion.

The composition transported probability density function (TPDF) method [2–4] is particularly attractive for the problem of soot production. In the TPDF method, single point statistics of thermochemical state variables are evaluated using transport equations for their joint probability density functions. The advantage of this approach is that processes which require only local information, such as the processes involved in soot formation and oxidation, appear in closed form [2]. Another advantage is that the TPDF method does not, at least formally, make any assumption of relative timescales of chemistry, which is attractive for turbulent flames involving soot that involve both fast and slow chemical processes.

The trade-off for avoiding the closure problem of chemical source terms in TPDF methods is that molecular micromixing becomes an unclosed term requiring modelling. For gas-phase species, much research has been devoted to mixing models, with commonly used approaches including the interaction by exchange with the mean (IEM) [5], modified Curl (MC) [6] and Euclidean minimum spanning tree (EMST) models [7]. These models have been compared in a number of experimental flame configurations [8–11].

The modelling of soot micromixing has received much less attention. Soot presents a problem in that it has a very high Schmidt number (order 10,000), and molecular transport is controlled mainly by thermophoretic velocities [12]. As a result, even in simple homogeneous mixing, soot is expected to have a different small-scale behaviour than typical gaseous species, for instance possibly exhibiting a viscous-convective subrange in its energy spectrum [13]. At sufficiently high Reynolds numbers (Re), such small-scale dissipative differences would not be expected to require corrections to mixing models in the case of non-reacting mixing, since the small scales adjust to large scales regardless of Sc. However, it is not clear that Re in typical combusting flows is sufficient to observe this limit, and in addition soot is coupled to small-scale chemical processes, which might not result in a vanishing differential diffusion effect even at very high *Re*. As such, the existing mixing models should be tested to determine whether they need improvement, and recommendations for how soot mixing should be treated need to be developed.

One approach to evaluate mixing models is by comparison to TPDF model outcomes to experimental data. Various TPDF models of turbulent experimental sooting flames have been reported, including ethylene-air nonpremixed jet flames [14, 15], a methane-air jet flame, [16], *n*-dodecane spray flames [17], etc. Among these studies, IEM was used in [18, 19], MC was used in [20, 21], and EMST was used in [22]. Soot mixing was typically treated the same as gas-phase species (apart from [22], in which soot was not mixed). To our knowledge, there have been no systematic comparisons of mixing models for sooting flames.

Despite the above contributions, the modelling of soot mixing is not a closed problem. Importantly, in comparisons to experimental work it is difficult to definitively isolate the effect of the molecular mixing model on the error, since there is also significant uncertainty in chemical mechanisms, soot mechanisms, and in the measurements themselves, as measurements are quite difficult compared with flames without appreciable soot. An alternative approach is the use of direct numerical simulations (DNS). In DNS, chemistry and soot mechanisms can be treated as known quantities, and "measurement" errors (i.e. numerical errors) can be made small. In fact, following the approach of Krisman et al. [23] and later Kuron et al. [24], sources of error can be further reduced by providing directly from the DNS the inputs that would normally required from a turbulence model, i.e. the mixing frequency, mean velocity, and turbulent diffusion coefficient.

Given this background, the objective of this study is to evaluate in the Reynolds-averaged composition TPDF framework how soot predictions are affected by the modelling of molecular mixing for the gas-phase species and soot, in order to provide guidance for model selection. In particular, we compare model outcomes from a TPDF code against DNS of a previously reported nonpremixed, turbulent, temporally evolving plane jet flame burning ethylene fuel. The DNS consider a 19 species chemical mechanism and soot is modelled using the Leung and Lindstedt model [25]. Three mixing models, IEM, MC and EMST are considered. To evaluate soot mixing we consider two extreme limits: either by not mixing soot at all, or in conjunction with EMST, mixing it in the same way as the gas-phase species. The TPDF code takes all inputs normally required from a turbulence model and uses the same sub-models as in the DNS, thus enabling a clear attribution of the success or failure of the model to the mixing models.

2. DNS configuration

Using the code S3D [26], the DNS modelled a temporally evolving nonpremixed plane-jet flame burning ethylene fuel. The simulation is described in Ref. [12] so only a brief summary is provided here. The configuration and parameters were chosen to maximise the Reynolds number while avoiding local extinction and ensuring a sufficient statistical sample with a reasonable computational effort. The DNS was initialised with a three-dimensional planar slab of fuel moving in a direction opposite to that of surrounding oxidiser streams on each side. In the fuel stream, the initial velocity was $\Delta U/2$, while it was $-\Delta U/2$ in the surrounding oxidiser streams, where ΔU was 82 m/s. The jet height, denoted H, was 1.8 mm. The jet Reynolds number, $Re_{jet} = 3700$, is defined as $Re_{jet} = \Delta U H / v_f$. Here v_f is the kinematic viscosity of the pure fuel stream. The initial mean velocity field was specified using hyperbolic tangent functions, to provide a smooth transition between the fuel and oxidiser streams. To trigger shear-generated turbulence, the mean velocity field was perturbed by homogeneous isotropic turbulence, having a constant intensity inside the jet and transitioning smoothly to zero in the oxidiser. The initial integral length scale, l_t , was equal to H/3, and the initial turbulence intensity, u' was equal to 4% of ΔU . The flame was initialised from a steady flamelet. The domain size was $16H \times 11H \times 6H$, and the resolution was $H/\delta x = 60$, selected to resolve properly both turbulence and flame structures [12]. The simulation was integrated up to 50 characteristic jet times $t_i = H/\Delta U$. A schematic diagram of the DNS configuration is presented in Figure 1. The fuel and oxidiser temperatures are both 550 K. To move the stoichiometric mixture-fraction into the shear layer and thus allow more turbulence-chemistry interaction, some nitrogen is moved from the oxidiser stream to the fuel stream while maintaining a constant stoichiometric flame temperature; see [12] for the detailed compositions.

The configuration permits the formation of a statistical ensemble by averaging in the stream-wise and spanwise directions and using symmetry in the transverse direction, y, leaving only a statistical dependence on y and time, t. The ensemble average is performed on a mass (Favre) basis, where the Favre-average of property ϕ , is



Figure 1: Visualisation of temporally evolving jet, coloured by the mixture fraction. Reproduced from Ref. [12].

defined as $\tilde{\phi} = \overline{\rho \phi} / \overline{\rho}$, where the over-bar represents a Reynolds-averaged quantity.

The soot mechanism is based on the approach of Leung *et al.* [25] and is described in full in Ref. [12], in this model, the soot is approximated by the solid carbon species, $C_{(s)}$. The soot mechanism is a 4 step mechanism, Eqs. (1-4) refer to the processes of nucleation, surface growth, oxidation and agglomeration used in this mechanism, respectively.

$$C_2H_2 \longrightarrow 2C(s) + H_2 \tag{1}$$

$$C_2H_2 + nC(s) \longrightarrow (n+2)C(s) + H_2$$
 (2)

$$C(s) + \frac{1}{2}O_2 \longrightarrow CO$$
 (3)

$$nC(s) \longrightarrow C_n(s) \tag{4}$$

The soot particle size distribution is modelled using the method of moments in which the first three mass moments of the particle size distribution are transported and closure of fractional moments in the chemical source term is performed by assuming a lognormal size distribution [27].

The DNS considered molecular mixing of soot via Brownian diffusion and thermophoresis, where the diffusion flux of soot, j_M , is given by:

$$j_M = -\rho D_p \nabla (\frac{1}{Le} \frac{M}{\rho}) - 0.554M \frac{\nu}{T} \nabla T$$
 (5)

where *M* is a soot moment (e.g. soot number density, soot mass density), D_p is the soot diffusivity, and v is the kinematic viscosity. In Eq. 5, since Le~10,000 [12], the first term (Brownian diffusion), while implemented, is negligible.

3. TPDF method

The composition TPDF approach in a Reynoldsaveraged framework is adopted. Equation 6 is the governing transport equation for the composition PDF [2]. Here \tilde{f}_{ϕ} represents the Favre-joint composition probability density function, \tilde{v}_j and v''_j are the Favre mean and fluctuation velocity components, respectively, ψ_{α} is the sample-space mass fraction and enthalpy, ω_{α} is the chemical source term, and J^{α} is the scalar flux tensor.

$$\frac{\partial}{\partial t} [\langle \rho \rangle \widetilde{f}_{\phi}] + \frac{\partial}{\partial x_{j}} [\langle \rho \rangle \widetilde{v}_{j} \widetilde{f}_{\phi}] + \langle \rho \rangle \frac{\partial}{\partial \psi_{\alpha}} [\omega_{\alpha} \widetilde{f}_{\phi}] = -\frac{\partial}{\partial x_{j}} [\langle \rho \rangle \langle v_{j}^{\prime \prime} | \psi_{\alpha} \rangle] \widetilde{f}_{\phi} + \frac{\partial}{\partial \psi_{\alpha}} \Big[\left\langle \rho^{-1} \frac{\partial J_{j}^{\alpha}}{\partial x_{j}} \middle| \psi_{\alpha} \right\rangle \langle \rho \rangle \widetilde{f}_{\phi} \Big] \quad (6)$$

The terms on the left hand side are closed and represent the temporal evolution, transport of the composition PDF in physical space due to the Favre-averaged velocity, and transport in composition space due to chemical reaction. The terms on the right hand side require modelling. The first term represents transport in physical space due to turbulent velocity fluctuations, and is closed here using a gradient diffusion hypothesis [28]. The second term represents the transport in composition space due to molecular diffusion; and the modelling of this term is the focus of this study.

The PDF transport equation is solved using the Monte Carlo method proposed by Pope [2] in the same way as in previous studies in our group [23, 24]. The method solves for a system of stochastic differential equations (given below) for the position and composition of notional particles whose PDFs evolve the same way as the modelled PDF transport equation.

$$dx(t) = \left[\widetilde{V} + \frac{\nabla \widetilde{\rho} \widetilde{\Gamma_T}}{\overline{\rho}}\right] dt + \sqrt{2\widetilde{\Gamma_T}} dW \tag{7}$$

$$d\phi(t) = [\mathbf{M}]dt + [\mathbf{R}]dt \tag{8}$$

Equation 7 represents the transport of particles in physical space. This equation is composed of a deterministic term, $\left[\widetilde{V} + \frac{\nabla \rho \widetilde{\Gamma_T}}{\overline{\rho}}\right] dt$, and a stochastic term, $\sqrt{2\widetilde{\Gamma_T}} dW$. The deterministic term represents the effect of the mean velocity field (\widetilde{V}) and turbulent diffusion velocity ($\frac{\overline{\rho} \nabla \widetilde{\Gamma_T}}{\overline{\rho}}$). The stochastic term models the turbulent transport of particles using a Wiener process having increment dW. Equation 8 represents the evolution of particles in composition space. The first term represents the effect of molecular mixing, and models for this term are discussed further below. All of the models depends functionally on a mixing frequency Ω . The second term represents the effect of chemical reaction, which is treated identically to the DNS and therefore does not need additional approximation.

The solution of Eqs. 7 and 8 requires some inputs that would normally be provided from a turbulence model, specifically the mean velocity, V, turbulent diffusivity, Γ_T , and mixing frequency Ω . Here, following Krisman et al. [23], to eliminate the turbulence model and the associated constants (turbulent Schmidt number and C_{ϕ}) as sources of error, these quantities are taken directly from the DNS. In principle, Γ_T and Ω could be determined in various ways. Here, because this is a nonpremixed flame, it is considered that correctly predicting the first and second moment of the mixture-fraction PDF is likely to provide the optimal results. Therefore, diffusivity is calculated in a way that will result in a correct turbulent flux of mixture fraction, i.e. $\widetilde{\Gamma_T} = \frac{\rho v \overline{z} - \rho v \overline{z}}{\rho \nabla \overline{z}}$, where ρ is the density, v is the velocity in the y direction and Z is the Bilger's mixture fraction. The mixing frequency is prescribed such that the scalar dissipation of mixture fraction matches the DNS, i.e. $\Omega = \widetilde{\chi_Z} / \widetilde{Z''^2}$, where $\widetilde{Z''^2}$ is the Favre-averaged variance of mixture fraction, and $\widetilde{\chi_Z}$ is the Favre-averaged scalar dissipation rate. The approximation $\widetilde{\chi_Z} = 2D|\nabla Z|^2$, where D is the thermal diffusivity, was found to be sufficiently accurate as judged by the temporal evolution of mixture fraction root mean square (RMS) profiles.

For the mixing model, in the next section we present results in which the gas-phase species are mixed with IEM, MC and EMST while soot is not mixed. Later, the EMST results without soot mixing are compared with those where soot moments are treated exactly the same as the gas phase within EMST.

For all simulations presented here, the number of cells used in the simulation (N_{cell}) is 384 and the number of particles per cell (N_{pc}) is 2000. These parameters were found to be large enough to ensure statistical convergence for the first and second moments.

Finally, we mention that in the DNS, radiation is also considered using an optically thin model. However, Lignell *et al.* [12] noted that radiation is insignificant; therefore it is not considered in this study.

4. Results

This section is organised as follows. The distributions of mixture fraction are compared between the TPDF simulations and the DNS to validate the TPDF implementation in Section 4.1. Following this, the TPDF results of flame dynamics and soot prediction are compared to those of the DNS in Section 4.2. In the TPDF, various mixing models of the gas phase are first considered while the soot mixing is neglected. Finally, the effect of soot mixing on the soot prediction is examined in Section 4.3 by comparing the TPDF results with and without soot mixing using the EMST model for the gas phase.

4.1. Mixture fraction

Figure 2 (top) presents the spatial profiles of mean mixture fraction at 30 and 50 t_j . These times are chosen as they occur well after the turbulence has fully developed. It is shown that all mixing models correctly predict the mean mixture fraction profile. Since the mean mixture fraction is only affected by particle transport, the results presented provide confidence that the gradient diffusion hypothesis is valid and the data needed for the TPDF simulations have been correctly extracted from the DNS.



Figure 2: Mean (top) and RMS (bottom) mixture fraction profile at 30 and 50 t_j .

Figure 2 (bottom) presents the spatial profile of RMS mixture fraction at 30 and 50 t_j. The performance of various mixing models is similar. Particularly, at 30 t_j the TPDF results with different mixing models slightly overpredict the peak RMS. The TPDF and DNS results agree better at 50 t_j. The overall good agreement between the TPDF and DNS profiles indicates that the mixing frequency in the TPDF simulation is appropriate. The difference observed in the RMS mixture fraction may be due to the fact that the turbulent Schmidt number required for transport of the variance is difference.

ent for that of the mean or that there is some influence of differential diffusion in the gas-phase species.

4.2. Flame dynamics and soot prediction

Figure 3 compares the spatial and temporal evolution of the mean temperature from the TPDF to that from the DNS. The mean temperature is reasonably predicted by the TPDF method with the EMST model, although it is slightly lower than in the DNS. In contrast, the IEM and MC models both overpredict the amount of extinction, resulting in lower temperatures compared to the DNS from 20 t_j untill the end of the simulation.



Figure 3: Temporal evolution of the mean temperature.



Figure 4: PDF of temperature conditional on the mixture fraction at $30t_j$. Red solid line represents the conditional mean taken from the DNS, green dashed line represents the model conditional mean.

To further understand the high level of extinction in the TPDF results with the IEM and MC models, the PDF of temperature conditional on the mixture fraction at 30 t_j is shown in Fig. 4. The results at 50 t_j are similar so that they are not shown here. Only one burning branch is observed in the DNS and the TPDF results with the EMST model. The conditional mean of the temperature is predicted well by the EMST model. The conditional fluctuations are, however, underpredicted as demonstrated by the narrow PDFs, which can be seen as a limitation of the EMST model [23]. In contrast, the TPDF results with the IEM and MC models exhibit two branches of burning and partial extinction, resulting in a conditional mean temperature that is lower than the DNS results. The present results are consistent with an earlier study for ethylene flames without soot [23]. In that study the IEM and MC models also overpredicted the amount of extinction.

Since soot formation strongly depends on the temperature, the soot formation predictions vary strongly depending on the mixing model used. As the IEM and MC models cannot accurately predict the mean temperature, they are not able to produce, even qualitatively, the correct soot formation rates. Therefore the results for the IEM and MC models will not be presented in the context of soot formation. Figure 5 shows the spatial and temporal evolution of the mean soot mass fraction (Y_{soot}) from the DNS and the TPDF method with the EMST model for the gas phase. It is seen that the TPDF method produces similar soot mass fraction results as that of the DNS in both space and time.



Figure 5: Spatial and temporal evolution of the mean soot mass fraction.

The conditional statistics are examined in order to further understand the performance of the TPDF method in predicting soot formation. Fig. 6 shows the PDF of soot mass fraction conditioned on the mixture fraction at 50 t_j . The soot mass fraction exhibits very large conditional fluctuations in the DNS as result of the high intermittency of soot formation. This large conditional fluctuation is also captured by the TPDF method. Recall that in Fig. 6 the soot mixing is neglected while the EMST model is used for the gas phase.

4.3. Soot mixing

As mentioned in the introduction, the effect of molecular mixing of soot on the soot prediction remains unclear. The assumption of no soot mixing seems valid



Figure 6: PDF of soot mass fractionconditioned on the mixture fraction at 50 t_j . Red solid line represents the conditional mean taken from the DNS, green dashed line represents the model conditional mean

due to the large Schmidt number of soot. Alternatively, it can be assumed that the soot moments mix at the same rate as the gas-phase species. These assumptions are contrasted in this section as two extremes of the treatment of soot mixing. Note that since the soot is in such a low concentration here, the soot mixing only affects the soot statistics and does not affect the temperature or other thermochemical variables. Therefore the gasphase results presented above will not change regardless of whether soot mixing is applied or not.

Figure 7 shows the mean and RMS soot mass fraction profiles of the TPDF simulations at 30 and 50 t_j . The DNS results are also plotted as a reference. For the mean profiles, it is clear that setting the mixing rate to zero for the soot allows the TPDF method to accurately capture the mean soot mass fraction profile. When mixed at the rate of the gas-phase species, the soot mass fraction is underpredicted over the whole domain.



Figure 7: Mean (top) and RMS (bottom) soot mass fraction profile at 30 t_j and 50 t_j for both mixing assumptions.

Concerning the RMS soot mass fraction results, it is seen that when the mixing rate is zero the RMS soot mass fraction is overpredicted by the TPDF method. When the mixing rate is equal to that of the gas-phase species, the RMS soot mass fraction is considerably underpredicted.

To further examine soot mixing, Fig. 8 shows the PDF of soot mass fraction conditioned on the mixture fraction. It is readily observed that when soot is mixed at the same rate as the gas-phase species, the conditional fluctuations of soot mass fractions essentially disappear, with the majority of the PDF mass concentrated at the conditional mean. This is the typical behaviour exhibited by the EMST mixing model. Without molecular mixing of soot, the conditional PDFs show larger similarity to the DNS, as already discussed in Fig. 6.



Figure 8: PDF of soot mass fraction conditioned on the mixture fraction at 30 t_j and 50 t_j for each mixing assumption. Red solid line represents the conditional mean taken from the DNS, green dashed line represents conditional mean taken from the TPDF simulations.

It is clear from the presented results that the soot moments do not mix at the same rate as the gas-phase species. It appears that assuming no soot mixing produces good results for both conditional and unconditional mean quantities of soot mass fraction. However, the RMS of soot mass fraction is overpredicted using this assumption. This may imply that soot mixing occurs, however, at a rate that is much less than the gasphase species.

5. Conclusions

An evaluation of mixing models was performed in the context of a Reynolds-averaged TPDF method. The DNS configuration of a sooting, turbulent non-premixed jet flame with ethylene as the fuel was considered. In the TPDF modelling the mean mixing frequency, mean velocity, and turbulent diffusion coefficient were taken directly from a DNS database, enabling the elimination of several possible sources of modelling error.

The mixing model of the gas phase was found to significantly impact the results. Concerning the unconditional means of temperature, the EMST mixing model performs better than the other models. Both the IEM and MC models predict large extinction, which is not present in the DNS. This highlights the importance of the mixing model in the correct prediction of the flame dynamics.

The effects of soot mixing on the soot prediction were explored using the EMST model for the gas phase. It was found that when the soot moments mix at the same rate as the gas-phase species, the TPDF results show significant differences from the DNS results. Assuming the soot moments do not mix produces good results for both unconditional and conditional mean quantities of soot mass fraction. However, the RMS soot mass fraction is observed to be overpredicted, while it is underpredicted considering soot mixing. This may imply the mixing rate for soot is non-zero but smaller than the gas phase mixing rate.

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