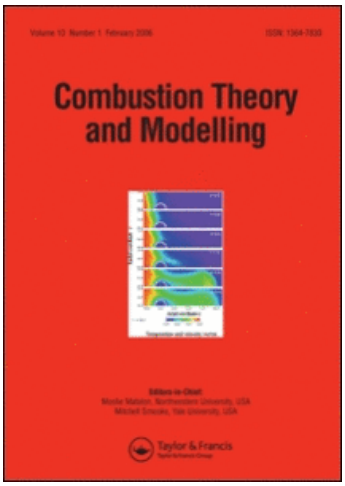

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Conditional velocity statistics in the double scalar mixing layer – A mapping closure approach

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In this work we use 3D direct numerical simulations (DNS) to investigate the average velocity conditioned on a conserved scalar in a double scalar mixing layer (DSML). The DSML is a canonical multistream flow designed as a model problem for the extensively studied piloted diffusion flames. The conditional mean velocity appears as an unclosed term in advanced Eulerian models of turbulent non-premixed combustion, like the conditional moment closure and transported probability density function (PDF) methods. Here it accounts for inhomogeneous effects that have been found significant in flames with relatively low Damköhler numbers. Today there are only a few simple models available for the conditional mean velocity and these are discussed with reference to the DNS results. We find that both the linear model of Kutznetzov and the Li and Bilger model are unsuitable for multi stream flows, whereas the gradient diffusion model of Pope shows very close agreement with DNS over the whole range of the DSML. The gradient diffusion model relies on a model for the conserved scalar PDF and here we have used a presumed mapping function PDF, that is known to give an excellent representation of the DNS. A new model for the conditional mean velocity is suggested by arguing that the Gaussian reference field represents the velocity field, a statement that is evidenced by a near perfect agreement with DNS. The model still suffers from an inconsistency with the unconditional flux of conserved scalar variance, though, and a strategy for developing fully consistent models is suggested.

Keywords: double scalar mixing layer, conditional mean velocity, conditional moment closure, turbulent mixing, direct numerical simulations

1. Introduction

In recent years we have seen major advances in the theoretical understanding and mathematical modelling of turbulent non-premixed combustion. The success is generally built on the observation that conserved and reactive scalars in turbulent non-premixed flames often are strongly correlated. Flamelet models [1] are derived by re-parameterizing the reactive scalar transport equations in terms of the conserved scalar, or mixture fraction, whereas the conditional moment closure [2] is derived by averaging the (conserved and reactive) transport equations conditioned on a value of this conserved scalar. Here the conditional mean velocity appears as an unclosed term accounting for inhomogeneities in the flame.

In many flames of commercial interest the conditional mean velocity is not of critical importance. In flames where the chemistry is fast compared to the rate of mixing (high Damköhler

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numbers) the only significant terms are the reaction rate and the scalar dissipation rate that exist in a pseudosteady state in localized flamelets. If the chemistry is not fast enough to immediately respond to mixing, other effects, like convective transport, become important. The conditional moment closure can offer significant improvements over simple flamelet models when such effects come into play. However, for improved predictions the conditional mean velocity needs to be modelled accurately and today there are only a few models available. Furthermore, these models have generally been validated in two-feed stream configurations [3–6] and little is known about the conditional mean velocity in more complex units commonly encountered in practical applications. The DSML is a canonical multistream flow and a model problem for the turbulent piloted diffusion flames forming a central theme in the international workshops on turbulent non-premixed flames [7]. The piloted diffusion flames now serve as a standard for which new models of turbulent non-premixed combustion are evaluated.

There are in general three well known models for the conditional mean velocity, the linear approximation of Kutznetzov and Sabelnikov [3] (modified versions exist), the Li and Bilger model [6] and Pope's gradient diffusion model [8]. The linear approximation is derived by making the assumption that the joint probability density function (PDF) of velocity and scalar is Gaussian. The model reads

$$\langle u_i' | \eta \rangle = \frac{\langle u_i' \xi' \rangle}{\langle \xi'^2 \rangle} (\eta - \langle \xi \rangle), \tag{1}$$

where u_i is a component of the velocity vector, ξ is a conserved scalar and η is a sample space variable for ξ. The prime is used to indicate fluctuation about the unconditional mean, which in turn is represented with the angle brackets. The linear model has been found to give an accurate representation of the conditional mean velocity in two-stream configurations for small $|\eta - \langle \xi \rangle|$. For large $|\eta - \langle \xi \rangle|$, though, deviations have usually been found significant even in simple scalar mixing layers [4, 6]. For multistream flows the joint velocity scalar PDF will be far from Gaussian and the model cannot be expected to perform well. Furthermore, the linear model is only consistent with traditional gradient diffusion modelling of the first moment of conserved scalars. Hence, the model is difficult to apply consistently with presumed PDF methods that also require the second moment. Note that extensions of the linear approximation exist, but these extended models have not found much use.

Li and Bilger [6] used a mixing length argument to explain the shortcomings of the linear model and derived a model tailored to scalar mixing layers

$$\langle u_i' | \eta \rangle = \langle u_i' | \eta = \langle \xi \rangle \rangle + \alpha \frac{u_{\mathrm{rms}}}{\delta} (y - y_\eta). \tag{2}$$

Here y is the transverse location of interest in the mixing layer (dimension in meter) and y_η is the location where the local mean mixture fraction is equal to η. u_{rms} is the root mean square velocity, α is a constant of order unity and δ is a length scale relevant to the flow. In the single scalar mixing layer (SSML) it was defined by Li and Bilger as the distance from where $\langle \xi \rangle$ was 0.1 to where it was 0.9. For a SSML the model (2) leads to a shape of the conditional mean velocity that is an inverse error function. This result is in close agreement with both experiments [6] and numerical simulations [4] of the SSML. An attractive feature of (2) is that it does not rely on a specific shape of $\langle \xi \rangle$ and in theory it should be equally valid for a double scalar mixing layer (DSML). We will investigate this in later sections. Unfortunately, there is no simple way of extending (2) to general geometries and the model is inconsistent with traditional gradient diffusion modelling of unconditional fluxes. This means that the model is difficult to use consistently in real applications.

Pope [8] made an analogy to traditional turbulent transport modelling and suggested a gradient diffusion model

$$\langle u_i' | \eta \rangle = -\frac{D_T}{p(\eta)} \frac{\partial p(\eta)}{\partial x_i}, \tag{3}$$

where D_T is the turbulent diffusivity and p is the conserved scalar PDF. Gradient diffusion modelling has traditionally received much criticism. Still, Equation (3) is the only model that is completely consistent with modelling of unconditional fluxes (both passive and reactive scalars) and the only model where conservation through transport is guaranteed (diffusion conserves the scalar). The accuracy of Popes' model will obviously depend on how well the scalar PDF represents the true PDF. Mortensen and de Bruyn Kops [9] showed that in a scalar mixing layer the β-PDF led to good agreement with direct numerical simulations (DNS). However, it was also found that, using the β-PDF, Equation (3) diverged rapidly to infinity at low probabilities (see Figure 3a in [9]). Mortensen and Andersson [10] used a presumed mapping function (PMF) approach for the PDF and obtained results superior to the β-PDF. More importantly, these authors showed that the model now was well behaved for the whole range of mixture fraction space, regardless of low probabilities. For both the β-PDF and the PMF-PDF the gradient diffusion model produced results closely resembling an inverse error function, as obtained in the experiments of Li and Bilger and in DNS [4]. Mortensen [9] and Sawford [11] have previously presented results for the conditional mean velocity in the DSML. Here it was shown that the conditional mean velocity was highly nonlinear and thus the linear approximation was found to perform poorly for all positions in the flow. Sawford also proved that the Li and Bilger model was better, even though it smeared out the nonlinearity too fast in comparison with DNS.

Due to the complexity of the gradient diffusion model, the linear approximation is often preferred in implementations of the conditional moment closure (CMC). The linear approximation is low cost and easy to use, but the conditional mean velocity is usually only linear within a short distance from $\langle \xi \rangle$. In this work we will suggest a new model that is comparatively simple to use and that still captures the nonlinearity of the velocity scalar correlations. We will then present DNS data for the conditional mean velocity in a DSML and discuss these results with respect to the model library.

This paper is organized as follows: in Section 2 the double scalar mixing layer is presented and details of the DNS are given. In Section 3 we summarize the application of presumed mapping functions for multistream mixing and give some useful analytical results for efficient implementations. A new model for the conditional mean velocity is introduced in Section 4 and the models are compared to DNS in Section 5. Final conclusions are made in Section 6.

2. The double scalar mixing layer

The DSML has been thoroughly investigated by Cha *et al.* [12], Mortensen *et al.* [13] and Sawford [11], where both mean fields and conditional statistics have been presented. For this reason we only find it necessary to give a brief summary here.

The DSML has three injection streams. The central pilot is premixed at stoichiometric composition, whereas the other two inlets contain either pure oxidant or pure fuel. The parameter $\langle D_n \rangle$ represents the local mean mass fraction of inlet stream n and is used by the presumed mapping function approach outlined in Section 3. The mean mixture fraction is given as a linear

combination of the three $\langle D \rangle$'s

$$\langle \xi \rangle = \sum_{n=1}^{3} \xi_n \langle D_n \rangle , \tag{4}$$

where we have used $\xi_n = 0, 0.25$ and 1 for inlet streams 1, 2 and 3 respectively.

Direct numerical simulations (DNS) of the DSML are performed using incompressible Navier–Stokes and scalar transport equations

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{5a}$$

$$\frac{\partial u_j}{\partial t} + u_i \frac{\partial u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{1}{\mathrm{Re}_0} \frac{\partial^2 u_j}{\partial x_i \partial x_i}, \tag{5b}$$

$$\frac{\partial \xi}{\partial t} + u_i \frac{\partial \xi}{\partial x_i} = \frac{1}{\mathrm{Re}_0 \mathrm{Sc}} \frac{\partial^2 \xi}{\partial x_i \partial x_i}. \tag{5c}$$

Throughout this paper the Einstein summation convention is implied by repeating Roman indices i, j and k. No summation is implied by other indices. Equations (5a)–(5c) have been non-dimensionalized by the initial integral length scale, L_0, and the initial rms velocity, u_0, so that $\mathrm{Re}_0 = u_0 L_0 / \nu$, where ν is the kinematic viscosity. $\mathrm{Sc} = 0.7$ is the Schmidt number. The simulations are those reported by Cha *et al.* [12]. Briefly, the velocity field is isotropic and homogeneous with an initial Reynolds number based on the integral length scale and the rms velocity of 374. The initial mixture fraction field has no fluctuations about the mean. Starting from these initial conditions, the governing equations are numerically solved using a pseudospectral technique to compute the spatial derivatives and a third-order fractional step method with pressure projection to advance the solution in time. The nonlinear term in the momentum equation is computed in rotational form and the corresponding term in the scalar equation is computed in conservation and convective form in alternating time steps in order to minimize aliasing. All of the fields are de-aliased at every time step using a spectral cutoff filter that removes energy in wavenumbers greater than 15/16 of the maximum wavenumber. Periodic boundary conditions are used in the stream- and spanwise directions, whereas free-slip conditions are specified in the direction of the mean scalar gradient. The numerical domain has 512^3 grid points.

The scalar field was allowed to evolve for six initial large-eddy turnover times. After the full simulation was run, the simulation was repeated from $t = 0$ to $t = 1.2$ with the centre of mixing layer located at five different y locations, and also with the layer flipped about $y = 0$ for another five simulations. This resulted in a total of 10 simulations of the mixing layer using the same velocity field. The process was repeated using a statistically similar velocity field to produce another 10 simulations. Furthermore, each simulation includes 512 xz-planes, each of which is treated as a separate realization of the layer. So the data reported for $0 \leq t \leq 1.2$ is from an ensemble average of 10240 realizations, while the data for $1.2 < t \leq 6$ is from 512 realizations.

To obtain $\langle \mathbf{D} \rangle$ and $\langle \xi'^2 \rangle$ (where a boldface font is used throughout this paper to represent a vector) we choose to employ a separate Reynolds averaged Navier–Stokes (RANS) code, taking merely the turbulent diffusivity and mixing time from the DNS. Note that this choice was made partly to be consistent with companion papers on the same data-set (Refs. [12] and [13]) where the DNS was used to compute only ξ and not the individual D's. It is also used because, from a modelers perspective, it is important to understand how a model can be used in practice. It would of course be a simple matter to run the DNS with two D's instead of ξ, but from experience we

know that RANS modelling of first moments is highly accurate in scalar mixing layers and this strategy also leads to completely smooth mean fields with easily obtainable gradients, required by (3). Diffusion in stream wise direction is neglected and the following dimensionless equation is solved for $\langle D_1 \rangle$ and $\langle D_3 \rangle$

$$\frac{\partial \langle D_n \rangle}{\partial t} = \mathcal{D}_T \frac{\partial^2 \langle D_n \rangle}{\partial y^2}, \tag{6}$$

where $\mathcal{D}_T$ is the turbulent diffusivity divided by $u0$ and $L0$. Boundary conditions are given in [13]. To close the mixture fraction PDF in Equation (10) we also need a separate transport equation for the variance. Note that there are only two independent $\langle D \rangle$'s as any one can be calculated from the other two as

$$\sum_{n=1}^{3} \langle D_n \rangle = 1. \tag{7}$$

The evolution of $\langle D_1 \rangle$, $\langle D_3 \rangle$ has earlier been presented in Figure 3 of [13] together with the implied $\langle \xi \rangle$ that also was compared to DNS. The excellent agreement justifies solving for merely ξ in the DNS. The evolution of the variance is given by Cha *et al.* [12] and it suffice to say that the agreement with RANS is comparable to that of $\langle \xi \rangle$.

3. The presumed mapping function

The presumed mapping function (PMF) approach utilizes the original mapping closure for homogeneous mixing [14] to arrive at formulas that can be used as presumed Eulerian mixing models for the mixture fraction PDF, conditional scalar dissipation rate (CSD) or conditional velocity. There is formally no difference from using another prescribed shape, like the β-PDF, Gaussian, etc., except from the fact that the shape is computed from prescribed initial conditions. Note that the PMF approach can be used to obtain realistic PDFs, etc. from any initial conditions (e.g. three inlet streams), whereas the β-PDF only is justifiable for binary mixing of two initially separated mixtures. This feature of the PMF approach makes it possible to find physically realistic Eulerian mixing models in highly complex flows.

Cha, de Bruyn Kops and Mortensen [12, 13] recently suggested a presumed mapping function approach that was shown to capture the fine-scale statistics in the DSML very well. The second paper also suggested a modelling strategy that could achieve this in a cost-efficient manner. A brief summary of this approach is given here, since it is necessary for the derivation of a cost-efficient recipe for the gradient diffusion model (3).

3.1. *Basic equations*

The mapping function X maps the unknown true scalar field to a known reference field. The mapping function used to describe multistream mixing can be found as

$$X(\phi, \mathbf{\Lambda}) = \xi_1 + \frac{1}{2}\left[\sum_{n=1}^{N-1} \triangle\xi_n \mathrm{erf}(\mathcal{F}_n) + \xi_N - \xi_1\right], \tag{8}$$

where

$$\mathcal{F}_n = \frac{\phi - z_n e^{\tau}}{\sqrt{2}\sigma}, \tag{9}$$

$\triangle\xi_n = \xi_{n+1} - \xi_n$ and $\sigma^2 \equiv e^{2\tau} - 1$ are used to simplify notations. Here the standard Gaussian $[p_\psi(\phi) = (2\pi)^{-1}\exp(-\phi^2/2)]$ is used as a reference PDF and ϕ is a sample space variable for the reference field ψ. Note that we need to order the inlet streams such that $\xi_{n+1} > \xi_n$. With knowledge of the mapping function, the PDF for multi stream mixing can be computed as [14]

$$p(X) = p_\psi(\phi)\left(\frac{\partial X}{\partial \phi}\right)^{-1}, \tag{10}$$

where the last terms can be obtained by a simple differentiation of (8) with respect to ϕ

$$\frac{\partial X}{\partial \phi} = \frac{1}{\sqrt{2\pi}\sigma}\sum_{n=1}^{N-1}\triangle\xi_n \exp\left(-\mathcal{F}_n^2\right). \tag{11}$$

In the inhomogeneous DSML there are three fixed parameters of X (and thus also of p) that are denoted as $\Lambda = [z_1, z_2, \tau]$. These parameters are closed in terms of the 'moments' of the PDF, i.e. $\boldsymbol{\mu} = [\langle D_1\rangle, \langle D_3\rangle, \langle\xi^2\rangle]$. The time parameter τ determines the evolution of mixing and z is algebraically related to $\langle \boldsymbol{D}\rangle$ through

$$z_n = \sqrt{2}\mathrm{erf}^{-1}\left(2\sum_{m=1}^{n}\langle D_m\rangle - 1\right). \tag{12}$$

To obtain the correct variance, the following equation must be solved for τ

$$0 = \langle\xi^2\rangle - \int_{-\infty}^{+\infty} X^2(\psi, \boldsymbol{\Lambda}) p_\psi d\psi. \tag{13}$$

3.2. *Computation of the conditional mean velocity*

Having decided on a form of the mixture fraction PDF, we are now ready to compute the gradient diffusion conditional mean velocity. Since p only is an indirect function of space and time, Equation (3) needs to be expanded as

$$\langle u_i'|\eta\rangle = -\mathcal{D}_T \frac{\partial \ln(p)}{\partial \Lambda_k}\frac{\partial \Lambda_k}{\partial \mu_j}\frac{\partial \mu_j}{\partial x_i}. \tag{14}$$

Note that this model only is valid for finite and non-zero p, which usually implies that $0 < \eta < 1$. For the DSML, though, it is more correct to set these limits as $D_1(x = 0) < \eta < D_3(x = 0)$. For the DSML there is also an intermediate value of η (in this work $\eta = D_2(x = 0) = 0.25$), where $p(\eta) \to \infty$ initially at high levels of segregation. In these limits of pure mixtures the model slowly approaches infinity (see Figure 3a in [9]). However, since no mixing has occurred at these extremes the conditional average concentrations solved for in CMC will here be known

and prescribed with Dirichlet boundary conditions. Hence, as long as the model is used with care within its valid range, it will not disturb regular CMC computations.

The last term in (14) is known from the solution of the moments (see Section 2), whereas the first two expansions generally can be found analytically. Note that the last two expansions merely are weights and hence it is only the first term that needs to be recomputed for each position in mixture fraction space. The simple analytical manipulations of the PDF is one of the major advantages of following the mapping closure approach and several recipes have already been provide in [10, 12, 13]. The analytical recipes required to implement the first term on the right hand side of Equation (14) efficiently are summarized in Appendix A.

The second expansion in Equation (14) is computed straight forward for z by differentiation of (12). However, the sign of the result will depend on which $\langle D \rangle$ that is chosen as the dependant. If we choose not to solve for stream q ($1 \leq q \leq N$) we obtain

$$\frac{\partial z_n}{\partial \langle D_m \rangle} = C\sqrt{2\pi}\exp\left(\frac{z_n^2}{2}\right), \tag{15}$$

where

$$C = \begin{cases} 1 & \text{for } m = n \text{ and } m < q \\ 0 & \text{for } m \neq n \text{ and } m < q \text{ or } m \neq n+1 \text{ and } m > q \\ -1 & \text{for } m = (n+1) \text{ and } m > q, \end{cases} \tag{16}$$

For τ it is somewhat more complicated since τ depends on all the parameters in $\boldsymbol{\mu}$. Hence both τ and $\partial\tau/\partial\mu_j$ must be found numerically for all j's. Considering the complexity that arise from the number of parameters it is important to remember that all recipes come with a negligible computational cost and the only computationally demanding task is still to obtain τ given $\boldsymbol{\mu}$ from Equation (13). If a good routine for finding τ is available, then it is also straightforward to compute the Jacobian $\partial\tau/\partial\mu_j$ in Equation (14) with finite differences. Note finally that it is of course also possible to approximate Equation (3) with finite differences in space. However, since p is only an indirect function of space and time, it is only the expanded version that will be completely consistent with the solution of $\boldsymbol{\mu}$. The approach outlined in this section is both robust and efficient in comparison even though the implementation time undeniably is higher.

4. A new model for the conditional mean velocity

Despite the efficient recipe given in Appendix 6 the gradient diffusion model is still somewhat complex and it might be of interest to find a simpler, even more cost-efficient model (at least in terms of implementation). Without much further discussion we suggest the following general statement as a starting point for modelling $\langle u_i' | \eta \rangle$

$$\langle u_i' | \eta \rangle = a_i \phi + b_i f(\phi). \tag{17}$$

Here a_i and b_i are weight parameters that need to be closed and $f(\phi)$ is simply a function of ϕ. Equation (17) is suggested mainly on empirical grounds, but a physical explanation will later be tried in terms of the mapping closure. The model is similar to Li and Bilger's, where the weight is determined by the rms velocity and a parameter of order unity. Here we will instead specify a_i and b_i in a consistent way such that $\langle u_i' \rangle = 0$ and the unconditional flux of ξ is obtained. In other

words we set the following constraints for computing a_i and b_i:

$$\langle u_i' \rangle = \int_0^1 [a_i \phi + b_i f(\phi)] p(X) dX$$
$$0 = \int_{-\infty}^{+\infty} [a_i \phi + b_i f(\phi)] p_\psi(\phi) d\phi \tag{18}$$

and

$$\langle u_i' \xi \rangle = \int_{-\infty}^{+\infty} [a_i \phi + b_i f(\phi)] X(\phi) p_\psi(\phi) d\phi. \tag{19}$$

Note that the parameters of X are already known and the integrals are without singularities. Hence the integrals are very easy to solve efficiently with most numerical integration routines. The average of p_ψ is zero and thus from the first constraint we obtain

$$b_i \int_{-\infty}^{\infty} f(\phi) p_\psi(\phi) d\phi = 0. \tag{20}$$

In this work we will use $b_i = 0$, which is the simplest possible model that satisfies (20). The model with $b_i = 0$ will from hereon will be denoted the reference field model. The second parameter a_i can now be computed as

$$a_i = \langle u_i' \xi \rangle \left(\int_{-\infty}^{+\infty} \phi X(\phi) p_\psi(\phi) d\phi \right)^{-1}. \tag{21}$$

By using $b_i = 0$ Equation (17) will not be consistent with the flux of mixture fraction variance. To find a model consistent with the flux of the variance, a non-zero b_i and thus a functional form of f is necessary. Here we will not try this extension, since the reference field model is still not well established. It suffice to say that [due to (20)] any odd function (e.g. $f = \phi^3$ or ϕp_ψ) will be a candidate for f.

Note that the reference field model not only is a model for DSMLs, but should be equally valid and simple to use for any configuration. For a general two-stream flow the model predicts an inverse error function shape of the conditional mean velocity, which is in close agreement with both experiments [6] and numerical simulations [4].

5. Results and discussion

In this section we present DNS results for the conditional mean velocity in the DSML and discuss the various models performance. The DSML near the two individual mixing layers (at y != ± 1 for small t) are similar to single scalar mixing layers that have been verified elsewhere [4, 5, 10]. Hence we choose to focus on the section of the DSML where there is significant contribution from all three inlet streams. Furthermore, we focus only on the velocity in the principal direction of change, which is the transverse. Figure 1 shows the conditional mean transverse velocity at several cross stream locations for $t = 0.8$ and 1.2. From Figure 1 it is possible to identify two separate inverse error function shapes (one for each region $0 - \xi_p$ and $\xi_p - 1$) that merges with time. The shape of the conditional velocity appears to be constant across the layer with merely a constant offset separating the curves at various y-locations.

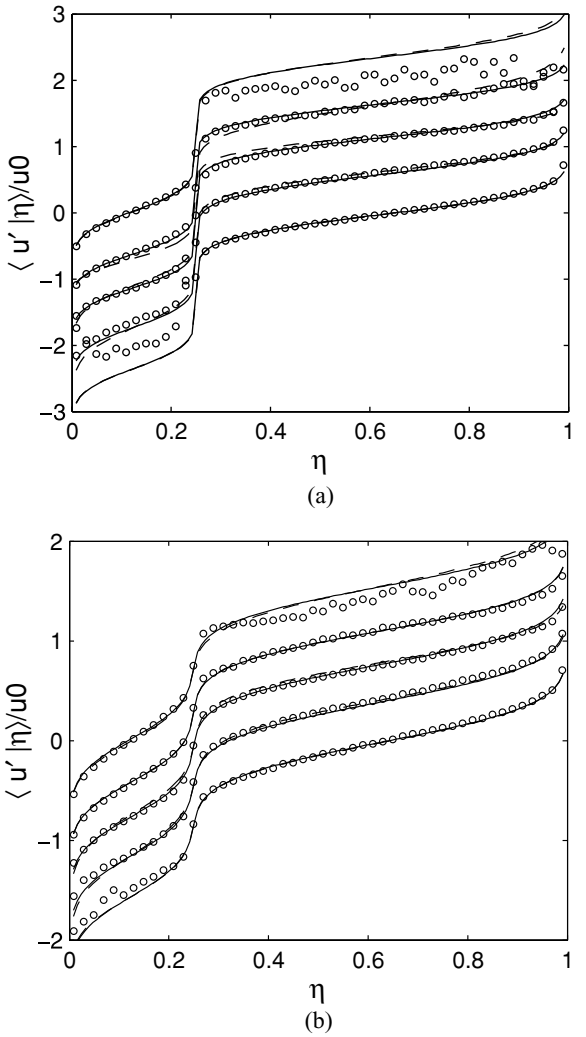

Figure 1. The conditional mean transverse velocity at $t = 0.8$ (a) and $t = 1.2$ (b). Positions of plots from top to bottom are $y = [1, 0.5, 0, -0.5, -1]$ in both figures. Circles, solid and dashed lines represent DNS, the reference field model and the gradient diffusion model respectively.

The highly nonlinear shape of the conditional mean velocity clearly shows that the linear approximation [Equation (1)] is unsuitable for multistream mixing. This has already been shown by Sawford [11] and thus the plot is not repeated here. It is possible to imagine an extended linear model, though, where one considers mixing to take place only between streams 1 and 2 or 2 and 3 leading to two linear profiles that are discontinuous at $\eta = \xi_2$. However, we do not think it's a good idea to spend time extending a model that has already been proven inaccurate for even simpler flows [4, 5]. Hence, this line of thought will not be followed any further.

The mean mixture fraction field is essential to the Li and Bilger model and this plot has already been presented in Figure 3(b) of Mortensen *et al.* [13]. From this figure it is evident that after one turnover time the central plateau has more or less disappeared and the DSML starts to resemble a single scalar mixing layer (SSML). The Li and Bilger model predicts a conditional

mean velocity that is proportional to the inverse of the mean field. Hence, according to this model the conditional mean velocity should be similar to a single inverse error function at $t = 1.2$. From this we can conclude that the conditional mean velocity is **not** proportional to the inverse mean scalar profile and the Li and Bilger theory gives poor predictions for the double scalar mixing layer. This is also evident from Figure 12 in [11]. The mean scalar profile describes macroscales in the flow. Since molecular mixing takes place at the finest scale of the flow, this disagreement is perhaps not surprising. The Li and Bilger model works well in a single scalar mixing layer where the flow is nearly self-similar and the shape of the mean profile remains constant throughout. In the DSML the shape of the mean profile evolves and quite clearly, the models theory is not of sufficiently fundamental character to capture this evolution at the correct rate. We can conclude that the Li and Bilger model merely is applicable for single scalar mixing layers.

The gradient diffusion [Equation (3)] and reference field [Equation (17)] models are compared with DNS in Figure 1. Both models are here seen to capture both the shape and the magnitude of the conditional mean velocity throughout the DSML and there are only minor differences between the two models. The only disagreement with DNS is found for $t = 0.8$ and $y = \pm 1$, in the regions where there are very low probabilities, p, and thus less accurate DNS statistics. Furthermore, it is likely that these observations correlate strongly with the largest scales in the flow since the largest eddies must be responsible for the bulk transport of scalars across the layers. Consequently, the DNS results at these low probabilities may be affected by boundary conditions or the largest wavenumber cutoff. Perhaps surprisingly, the simplest model, Equation (17), shows somewhat better agreement with DNS. It is very interesting to note that the conditional velocity is almost perfectly proportional to ϕ, which is exactly the model (17) with $b_i = 0$. Next we will try to present a physical interpretation of this result.

Consider a single one-dimensional diffusion layer, where ξ is a conserved scalar and x is space. The scalar ξ will obey the diffusion equation, which is identical to the mapping equation (see Ref. [10]). In the 1D lamella the PDF of ξ can be represented as

$$p \propto \frac{\partial x}{\partial \xi}, \tag{22}$$

which is exactly the mapping closure with a constant reference field. Since (22) is the solution to both the constant reference field mapping closure and the diffusion layer it can be argued that all diffusion effect are accounted for in the gradient of X, whereas the reference field accounts for turbulence and convection. The DNS in this work utilizes a homogeneous isotropic velocity field that itself has a Gaussian distribution. If we assume that the reference field used by the mapping closure is exactly this velocity field, then we would have $\langle u_i' | \eta \rangle = \phi$. Since we are using a standard Gaussian we obtain instead $\langle u_i' | \eta \rangle \propto \phi$, which is the proposed model. Note that if this explanation proves to be correct, then Equation (17) should be expected to perform worse for velocity fields that are significantly non-Gaussian. To further illustrate the correlation with velocity, we plot in Figure 2 the normalized root mean square velocity u_{rms} and the parameter a_i for some positions in the layer. It is quite obvious that a_i scales directly with u_{rms}. In fact, replacing the models constant in (21) with a simple $a_i = 0.84 u_{\mathrm{rms}}$ leads to results that are inseparable from those shown in Figure 1. However, the form given in (21) is more general and should be used in other configurations.

The reference field model is inconsistent with the unconditional flux used to compute the variance in the RANS code. To investigate the importance of this inconsistency, we have computed $\langle u \xi'^2 \rangle$ from the model and compared to the RANS flux. We find that the implied flux is within 2 % of the RANS for all times and locations within $y = \pm 2$. Hence, the error introduced through (17) should only be of minor importance in the DSML. Note finally that the reference field model

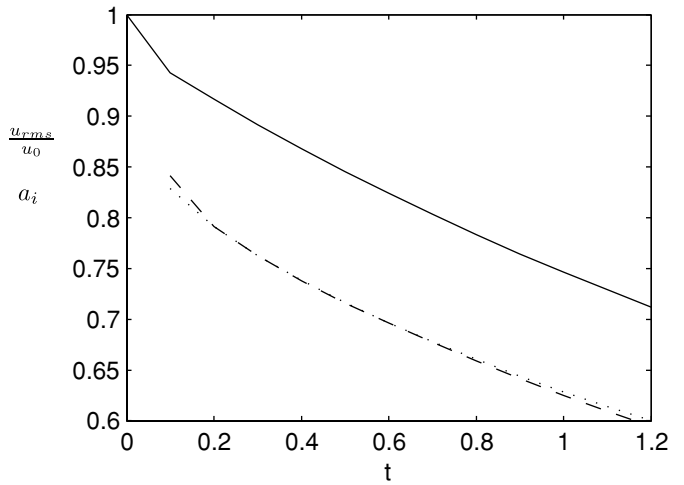

Figure 2. The solid line represents a normalized u_{rms} and a_i in Equation (21) is represented with a dashed and dotted line for $y = 1$ and -1 respectively.

gives predictions in a single scalar mixing layer that are equally convincing as for the DSML. These results are not reported, but should be evident from the inverse error function shape of the results given by Ref. [4].

6. Conclusions

In this work we have used 3D DNS to study a double scalar mixing layer (DSML), which is a model problem for piloted diffusion flames. The DSML has three separate injections with three different concentrations of a conserved scalar. This leads to complex shapes of the conserved scalar fine-scale statistics, important for models of turbulent non-premixed combustion. We have here focused on the average velocity statistics conditional on the conserved scalar that appears both in the conditional moment closure and in full PDF methods.

We identify that the complexity introduced by multiple injections cannot be captured by simplified models, such as the linear approximation and the Li and Bilger model. The gradient diffusion model still performs well, though, since it is based on the conserved scalar PDF that contains the fine-scale statistics of the flow. We give a brief discussion on the application of this model with the presumed mapping function approach of Cha *et al.* [12, 13] and derive several useful recipes for efficient implementations.

A new model for the conditional mean velocity, the reference field model, is suggested by utilizing the mapping closure reference field. We argue that the Gaussian reference field used by the mapping closure represents the velocity field, a statement that is evidenced by a near exact agreement with DNS. The model is much simpler to use than the gradient diffusion model and shows slightly better agreement with DNS. Furthermore, the model is of general nature and thus not only applicable to DSMLs. A drawback is that the model in its current form only is consistent with the unconditional flux of the first moment of the conserved scalar. For the DSML we find this inconsistency only leads to minor errors though. The reference field model should be able to simplify conditional moment closure codes and the extension to handle reactive flows will be investigated in future works.

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Appendix: A recipe for computing Equation (3)

In this appendix we manipulate the PMF-PDF to obtain a cost-efficient recipe for computing (3).

Using (10) the first derivative in Equation (14) can be rewritten on vector form as

$$\frac{\partial \ln p}{\partial \mathbf{\Lambda}} = -\phi \frac{\partial \phi}{\partial \mathbf{\Lambda}} - \left(\frac{\partial X}{\partial \phi}\right)^{-1} \frac{\partial^2 X}{\partial \mathbf{\Lambda} \partial \phi}. \tag{A1}$$

The derivative of ϕ with respect to $\mathbf{\Lambda}$ can then be found by considering Equation (8) at constant X and we obtain

$$\frac{\partial \phi}{\partial z_m} = \frac{1}{\sqrt{2\pi}\sigma} \left(\frac{\partial X}{\partial \phi}\right)^{-1} \triangle \xi_m \exp\left(\tau - \mathcal{F}_m^2\right), \text{ for } m < N \tag{A2a}$$

and

$$\frac{\partial \phi}{\partial \tau} = \phi + \frac{1}{\sqrt{\pi}\sigma^2} \left(\frac{\partial X}{\partial \phi}\right)^{-1} \sum_{n=1}^{N-1} \triangle \xi_n \mathcal{F}_n \exp\left(-\mathcal{F}_n^2\right). \tag{A2b}$$

Note that there is no summation implied by repeating m's. The last term of Equation (A1) can be written as

$$\frac{\partial^2 X}{\partial \mathbf{\Lambda} \partial \phi} = \frac{1}{\sqrt{\pi}} \sum_{n=1}^{N-1} \triangle \xi_n \exp\left(-\mathcal{F}_n^2\right) \left[\frac{\partial^2 \mathcal{F}_n}{\partial \mathbf{\Lambda} \partial \phi} - 2\mathcal{F}_n \frac{\partial \mathcal{F}_n}{\partial \mathbf{\Lambda}} \frac{\partial \mathcal{F}_n}{\partial \phi} \right]. \tag{A3}$$

All the terms on the right hand side can be found analytically. Differentiation of (9) leads to

$$\frac{\partial \mathcal{F}_n}{\partial \phi} = \frac{1}{\sqrt{2}\sigma}, \tag{A4a}$$

$$\frac{\partial \mathcal{F}_n}{\partial \tau} = \frac{1}{\sqrt{2}\sigma} \left(\frac{\partial \phi}{\partial \tau} + \frac{z_n e^{\tau}}{\sigma^2} - \frac{\phi}{a^2} \right), \tag{A4b}$$

$$\frac{\partial \mathcal{F}_n}{\partial z_m} = \frac{1}{\sqrt{2}\sigma} \left(\frac{\partial \phi}{\partial z_m} - e^{\tau} \delta_{m,n} \right), \text{ for } m < N, \tag{A4c}$$

$$\frac{\partial^2 \mathcal{F}_n}{\partial z_m \partial \phi} = 0, \text{ for } m < N \tag{A4d}$$

and

$$\frac{\partial^2 \mathcal{F}_n}{\partial \tau \partial \phi} = \frac{-1}{\sqrt{2}\sigma a^2}. \tag{A4e}$$

Here $a^2 \equiv 1 - e^{-2\tau}$ and $\delta_{m,n}$ is the Kronecker delta, that is unity for $m = n$ and zero for $m \neq n$. Inserting for Equations (A4a)–(A4e) into (A3) leads to further trivial simplifications.