PDF-Based LES Transport Models for Turbulent Reacting Flows

R. O. Fox[1] and V. Raman[2]

[1]Department of Chemical Engineering, Iowa State University, Ames, IA

[2]Center for Turbulence Research, Stanford University, Stanford, CA

Transported probability density function (PDF) methods offer many advantages, including the ability to treat the chemical source term exactly, but their computational cost is relatively high compared to other methods. In the context of Reynolds-averaged Navier-Stokes (RANS) simulations, this additional cost is often justified by superior predictions for reacting flow problems. However, when coupled with large-eddy simulations (LES) the additional cost (although independent of Reynolds number) may be prohibitive, and perhaps unjustified by the improvement in accuracy over competing methods. Nevertheless, the PDF transport equation (for both RANS and LES) offers a fundamental starting point for deriving simpler transport models that retain many of the desirable properties of transported PDF methods [Fox (2003)]. We have recently developed two such models: (1) the multi-environment PDF (MEPDF) model [Fox (2003)] and (2) the multi-environment conditional PDF (MECPDF) model [Fox & Raman (2003)]. Both models are based on presumed forms for the joint composition PDF:

$$f_{\boldsymbol{\phi}}(\boldsymbol{\psi}) = \sum_{n=1}^{N} p_n \delta\left(\boldsymbol{\psi} - \overline{(\boldsymbol{\phi})}_n\right) \text{ (MEPDF)}, \quad f_{\boldsymbol{\phi}|\boldsymbol{\xi}}(\boldsymbol{\psi}|\boldsymbol{\zeta}) = \sum_{n=1}^{N} p_n \delta\left(\boldsymbol{\psi} - \overline{(\boldsymbol{\phi}|\boldsymbol{\zeta})}_n\right) \text{ (MECPDF)}, \tag{1}$$

where $\boldsymbol{\phi}$ is the composition vector and $\boldsymbol{\xi}$ is the mixture-fraction vector. These models were first proposed by Fox (1998) as an inexpensive alternative to transported PDF simulations.

By inserting either of the presumed PDFs in Eq. 1 into a *closed* composition PDF transport equation, the direct quadrature method of moments (DQMOM) [Marchisio & Fox (2003)] can be used to find transport equations (RANS or LES) for the weights $p_n(\mathbf{x}, t)$ and the nodes $\overline{(\boldsymbol{\phi})}_n(\mathbf{x}, t)$ or $\overline{(\boldsymbol{\phi}|\boldsymbol{\zeta})}_n$. For example, for the MEPDF model the conservative forms of the LES transport equations are

$$\frac{\partial \overline{\rho} p_n}{\partial t} + \frac{\partial \overline{\rho} p_n \overline{U}_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\Gamma_{sgs}\frac{\partial p_n}{\partial x_i}\right) + \overline{\rho} a_n \tag{2}$$

and

$$\frac{\partial \overline{\rho} p_n \overline{(\boldsymbol{\phi})}_n}{\partial t} + \frac{\partial \overline{\rho} p_n \overline{(\boldsymbol{\phi})}_n \overline{U}_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\Gamma_{sgs}\frac{\partial p_n \overline{(\boldsymbol{\phi})}_n}{\partial x_i}\right) + \overline{\rho} p_n \mathbf{S}(\overline{(\boldsymbol{\phi})}_n) + \overline{\rho}\mathbf{b}_n, \tag{3}$$

where Γ_{sgs} is the subgrid-scale (SGS) turbulent diffusivity, $\mathbf{S}$ is the chemical source term, and a_n and $\mathbf{b}_n$ are the micromixing terms derived from DQMOM. As described in Fox (2003), the micromixing terms ensure that the first N moments of each component ϕ_α of the composition vector obey the corresponding transport equations. Thus, for example, with $N = 2$ the resolved scalar mean $\overline{\boldsymbol{\phi}}$ and SGS scalar variance found from the MEPDF model will obey the correct LES transport equations. The models are also adaptive in the sense that increasing N will increase the accuracy of the predictions. Indeed, for RANS calculations we have recently shown that they approach the predictions of transported PDF simulations for relatively small N [Wang & Fox (2003)]. Moreover, the computational cost of solving the MEPDF model for the same number of scalars is only a fraction of the cost of transported PDF simulations.

In this work, a two-environment MEPDF model was implemented in an LES code, and a constant-density reacting shear layer was simulated for a one-step reaction. Two scalars were required: ξ, mixture fraction; and Y, progress variable. A transported composition large-eddy PDF code was run for the same system and used to validate the MEPDF model. In general, the agreement between the two models is very good. Sample results are shown in Fig. 1 where it can be seen that the time-averaged mean and variance predictions from both models are very close, even though N is only two. Analogous agreement is seen for the moments of the mixture fraction, and higher-order moments of the progress variable. Implementation of the MEPDF model in the LES code for this example is straightforward, and involves the addition of five scalar transport equations. Since $p_1 + p_2 = 1$, Eq. 2 is solved for $n = 1$ with $a_1 = 0$. Equation 3 is solved for $n = 1, 2$ and $\alpha = \xi, Y$, for a total of four equations. For the two-environment model, the DQMOM terms in Eq. 3 are

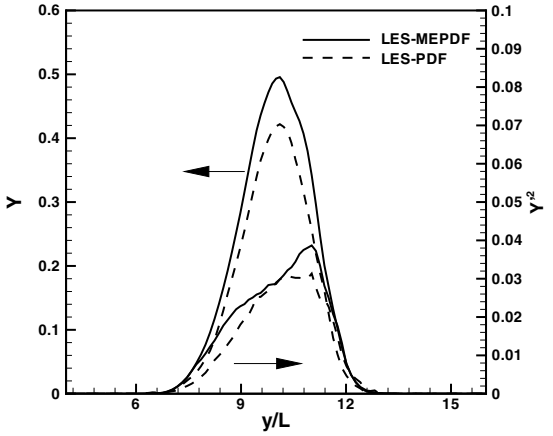

Figure 1: LES-MEPDF and transported LES-PDF results for the mean and the variance of the progress variable in a reacting shear layer.

$$b_{\alpha 1} = -b_{\alpha 2} = \frac{c_{\alpha 1} + c_{\alpha 2}}{\overline{(\phi_\alpha)}_1 - \overline{(\phi_\alpha)}_2} - \frac{p_1 p_2}{2\tau_\phi}\left[\overline{(\phi_\alpha)}_1 - \overline{(\phi_\alpha)}_2\right], \tag{4}$$

where τ_ϕ is the micromixing time scale and

$$c_{\alpha n} = p_n \Gamma_{sgs} \left(\frac{\partial \overline{(\phi_\alpha)}_n}{\partial x_i} \right)^2 . \tag{5}$$

The term involving $c_{\alpha n}$ in Eq. 4 functions as the source term for the scalar variances. The term involving τ_ϕ is the IEM micromixing model, and controls the scalar variance decay. For non-premixed reactants in the limit $\tau_\phi = \infty$, $\mathbf{b}_n = \mathbf{0}$ and the chemical source term in Eq. 4 is null. For this case, $\overline{(\boldsymbol{\phi})}_n$ will be constant and p_1 quantifies the degree of mixing between the two inlet streams.

The MECPDF model extends the MEPDF model by including transport terms in mixture-fraction space. When $N = 1$, the MECPDF model is formally equivalent to the conditional moment closure (CMC) [Klimenko & Bilger (1999)]. When $N = 2$, the MECPDF model provides a description of the conditional variance $\langle Y''^2 | \xi \rangle$. Higher-order conditional moments can be modeled by increasing N. As time allow, preliminary results for homogeneous mixing and the reacting shear layer found using the MECPDF model will be presented.

References

Fox, R. O. 1998 On the relationship between Lagrangian micromixing models and computational fluid dynamics. *Chemical Engineering and Processing* **37**, 521–535.

Fox, R. O. 2003 *Computational Models for Turbulent Reacting Flows*. Cambridge: Cambridge University Press.

Fox, R. O. & Raman, V. 2003 Multi-environment conditional PDF model In preparation.

Klimenko, A. Y. & Bilger, R. W. 1999 Conditional moment closure for turbulent combustion. *Progress in Energy and Combustion Science* **25**, 595–687.

Marchisio, D. L. & Fox, R. O. 2003 Direct quadrature method of moments: Derivation, analysis and applications. *Journal of Computational Physics* In review.

Wang, L. & Fox, R. O. 2003 Comparison of micromixing models for CFD simulation of nanoparticle formation by reactive precipitation. *AIChE Journal* In review.