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Numerical Implementation of Molecular Transport and Mixing in LES/FDF of Turbulent Flows SHARADHA VISWANATHAN, STEPHEN POPE — In large-eddy simulations of turbulent flames, the effect of molecular diffusion on scalar transport is significant and therefore needs to be modeled correctly in Lagrangian Filtered Density Function (FDF) methods. McDermott *et al.* (2007) show that in FDF methods, modeling molecular diffusion as a mean drift term in the scalar equation avoids the spurious production of scalar variance. Following McDermott *et al.*, we incorporate the effects of molecular diffusion in the Interaction by Exchange with the Mean (IEM) mixing model. In this study, we evaluate two second-order-accurate numerical methods *viz.* Particle-In-Cell (PIC) and Cloud-In-Cell (CIC) for implementing mixing. Given the nominal particle number density and problem geometry in a typical FDF calculation of a jet flame, the estimated mean field needs to be smoothed both for variance reduction and for proper treatment of empty cells near the jet axis. Our numerical studies show that while both implementations achieve detailed conservation and guarantee boundedness of the scalar field, CIC is computationally expensive and PIC is dependent on the scalar bounds. But for a given accuracy, PIC with smoothing incurs typically half the cost of CIC, for an appropriate choice of the smoothing parameter. This research is supported by the Department of Energy under Grant No. DE-FG02-90ER.

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