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A particle formulation for treating differential diffusion in filtered density function methods R. MCDERMOTT, S. B. POPE, Cornell University — We present a new approach for treating the molecular diffusion term in filtered density function (FDF) methods for modeling turbulent reacting flows. The diffusion term accounts for molecular 'transport' in physical space and molecular 'mixing' in scalar space. Conventionally, the FDF is represented by an ensemble of fluid particles and transport is modeled by a random walk in physical space. There are two significant shortcomings in this transport model: (1) the resulting composition variance equation contains a spurious production term, and (2) because the random walk is governed by a single diffusion coefficient, the formulation cannot account for differential diffusion, which can have a first-order effect in reacting flows. In our new approach transport is simply modeled by a mean drift in the particle composition equation. The resulting variance equation contains no spurious production term and differential diffusion is treated easily. Hence, the new formulation reduces to a DNS in the limit of vanishing filter width, a desirable property of any LES approach. We use the IEM model for mixing. It is shown that there is a lower bound on the specified mixing rate such that the boundedness of the compositions is ensured. We also present a numerical method for solving the particle equations which is second-order accurate in space and time, obeys detailed conservation, enforces the boundedness constraints, and is unconditionally stable.

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