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A MIXING MODEL TO IMPROVE THE PDF SIMULATION OF TURBULENT DIFFUSION FLAMES

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A new mixing model based on Euclidean minimum spanning trees (EMST), which has been developed by Subramaniam and Pope, is used in the PDF simulation of pilot-stabilized turbulent non-premixed flames. A model equation is solved for the joint PDF of velocity composition and turbulence frequency using a particle mesh method. Simulations using the EMST mixing model and the IEM (interaction by exchange with the mean) mixing model are compared. A simple thermochemistry equivalent to one-step reaction is used in the calculations. Comparisons are made with experimental measurements in the upstream regions of piloted H_2/N_2 flames. This fuel is chosen because its chemistry is simple and may be adequately represented by a single-step mechanism. It is found that the EMST model gives the correct mixing pattern for the reactive scalar, as well as the conserved scalar, especially in the early parts of the jet where mixing is most difficult to represent. This result is not achieved by the IEM model. The success of the EMST mixing model is attributable to its satisfying a "localness" condition that other models violate. This is a significant advance that will enable the PDF approach to simulate complex flows with finite rate chemical kinetics.

Introduction

The main advantage of using the joint PDF approach in the simulation of turbulent combustion lies in its capability to represent chemical reaction exactly. However, the accuracy of the approach depends also on the modeling of molecular mixing. In reacting flows, mixing of both reactive and conserved scalars occurs and modeling such processes must be adequate, particularly if finite-rate chemistry effects are involved. This is especially important close to the exits of fuel and pilot jets, where the gradients are steep and the scalars are evolving in time under significant turbulent mixing rates. It is also important at the base of lifted flames. Some previous attempts to compute the structure of pilot-stabilized non-premixed flames close to blow off have not been successful despite the use of realistic chemistry [1]. This is mainly due to the fact that just downstream of the pilot flame gases, mixing of reactive scalars is incorrectly represented, leading to largely nonreactive fluid mixtures that prevent ignition further downstream.

Central to the development of mixing models are important questions about how multiscalar mixing occurs. The simple particle interaction model developed by Curl [2] has undergone various modifications [3,4] and has been used with limited success [5]. The IEM model developed by Dopazo [6] represents a significant improvement in computing the structure of turbulent pilot-stabilized flames [4]. Both Curl's model and the IEM model perform poorly on the simple test case of a conserved scalar decaying to Gaussian in homogeneous, isotropic turbulence [7]. But for inhomogeneous flows, the production of scalar fluctuations by mean gradients ameliorates this deficiency. More important in the present context is that neither model satisfies the "localness principle," namely that mixing occurs locally in composition space [4]. Mapping closure methods [8] give excellent results for the simple test cases and satisfy the localness principle. Although there have been various efforts to extend this approach to multiscalar mixing [9,10–12], significant problems are encountered, particularly in its numerical implementation. The linear eddy mixing approach developed by Kerstein [13–15] shows promising results and has the unique advantage of being capable of accounting for differential diffusion ef-

fects. It has been used by Menon et al. [16] to compute the structure of jet flames.

The issue of multiscalar mixing remains unresolved and is the subject of intense research. Recently, a mixing model based on EMST has been developed by Subramaniam and Pope [17]. The EMST is used to identify neighboring fluid particles in composition space, and mixing then occurs only between these particles. The model satisfies Pope's rules of boundedness [18] and localness [4]. A version of the model that satisfies Pope's linearity principle [18] has also been developed but is not used in this paper. The model has been validated satisfactorily with the simple test problems of multiple scalars decaying in homogeneous isotropic turbulence and the evolution of a scalar field in an imposed mean scalar gradient. Further details about the model, its performance, and its convergence and numerical characteristics may be found elsewhere [17].

The purpose of this paper is to demonstrate that the new EMST mixing model gives a realistic representation of mixing in the early region of pilot-stabilized flames. This is particularly important for obtaining the correct flame structure further downstream. The model is coupled to a new stand-alone PDF code developed for two-dimensional turbulent reacting flows [19]. The joint PDF of velocity composition and frequency are solved using the particle–mesh method. The single-step chemistry used in these simulations is rather simple but is adequate to demonstrate the different performance of the mixing models. The reaction rate is a function of mixture fraction, ξ, and a reaction progress variable, b. Computations using both the EMST and IEM mixing models are compared with experimental measurements in a pilot-stabilized turbulent diffusion flame of H_2/N_2 fuel mixture.

Numerical Considerations

The PDF Code

The approach is based on the transport equation for the joint PDF of velocity, composition, and turbulent frequency. A Lagrangian method is used to solve the Eulerian PDF transport equation, and stochastic models are used for the velocity, dissipation, and molecular mixing terms. The evolution of the fluid particle velocity is represented by the simplified Langevin model [7], and a new stochastic model for turbulent frequency is employed [20]. Constants $C_{\omega 0}$, $C_{\omega 1}$, and C_ϕ in the turbulent frequency and composition equations are valued at 2.1, 0.04, and 2.00, respectively. The sensitivity of the solution to these constants is yet to be investigated, but Norris and Pope [21] have found that a higher value of $C_{\omega 0}$ is more appropriate for axisymmetric jets. The scalar mixing models are addressed in the next subsection.

The new code solves the PDF equations for two-dimensional flows and uses a particle–mesh numerical method [19]. A rectangular grid is used, and the mean properties are determined for each grid node. The instantaneous properties are carried by stochastic particles within each cell. The code can and has been implemented with parallel processing. This facilitates accurate calculations with many particles in a reasonable amount of elapsed time. Although used here for parabolic flows, the main virtue of this new code is that it allows, for the first time, the use of full PDF approach to compute the structure of recirculating flows.

The Piloted Flame

The pilot-stabilized burner has been used extensively as a model problem for simple parabolic flows with small and extreme departures from chemical equilibrium. The burner consists of a central fuel tube 7.2 mm in diameter, surrounded by an 18-mm annulus for the premixed flame pilot. A large body of experimental data is available for piloted flames over a range of fuel mixtures [22]. The initial and boundary conditions for the flames are well-known and these are described elsewhere [5]. To validate the numerical simulations, pilot-stabilized flames of H_2/N_2 (1/1 by vol.) fuel are investigated experimentally. Joint images of temperature and mixture fraction are collected in these flames just downstream from the jet exit plane. The Raman–Rayleigh technique, which is fully described elsewhere [23], is used for these measurements. Hydrogen-nitrogen fuel is used because it has moderately fast chemistry and the dilution with nitrogen increases the stoichiometric mixture fraction to $\xi_s = 0.305$ and forces the reactive zone into the shear layer. Measurements are taken in the region in which the pilot stream is still separating the fuel and airstream and further downstream in the region where fuel, air, and pilot gases are mixing together.

The Thermochemistry

Detailed chemical kinetics may be implemented easily in the PDF code and are not required here since only fast chemistry is considered. A very simple thermochemical model that simulates one-step chemical reaction is used in the simulations. The reaction rate is given as a function of two variables (ξ and b), where b is a reaction progress variable that varies from 0 for fully frozen to 1 for fully reacted fluid particles. Four parameters are needed to specify the reaction rates: a stoichiometric mixture fraction, ξ_s, a chemical time scale, τ_c, the curvature of the progress variable in mixture fraction space, at equilibrium, $\Delta\xi_e$, and a rich mixture fraction limit, ξ_r. The thermochemistry is self-similar and may be applied over a range of ξ_s values. Figure 1 shows

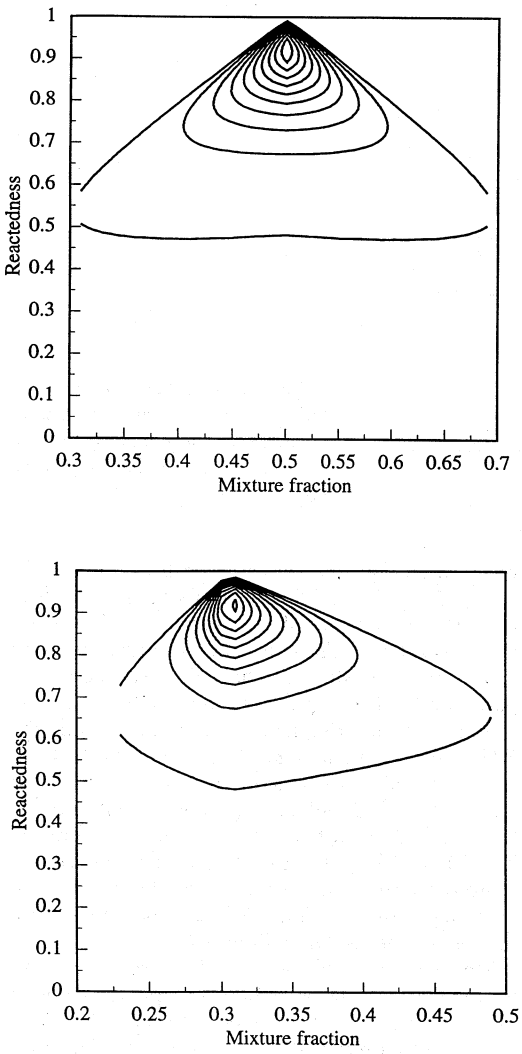

FIG. 1. Contours of normalized reaction rate plotted with respect to reaction progress variable b and mixture fraction ξ for two fuels with stoichiometric mixture fractions $\xi_s = 0.305$ and 0.5.

contour plots of the rates obtained for two "fuels" with $\xi_s = 0.305$ and 0.5, respectively. The first stoichiometry ($\xi_s = 0.305$) matches the H_2/N_2 fuel mixture for which experimental data are presented here. The case of $\xi_s = 0.5$ is used because the chemistry is symmetric, as shown in Fig. 1. The nonlinearity of the rates for all "fuels" is obvious and the modeled rate function peaks closer to stoichiometric, which is consistent with actual chemical kinetic rates. The lean and rich reactive limits, ξ_L, ξ_R are set where the rate drops to 1% of the peak value, and the contours shown in Fig. 1 are limited to this range. The chemical parameters used here for both "fuels" are $\tau_c = 2.0 \times 10^{-9}$ and $\Delta\xi_e = 1.0 \times 10^{-3}$. This corresponds to a chemical timescale that is short enough to simulate the fast chemistry studied in this paper and represented by the H_2/N_2 fuel mixture. More details on this self-similar thermochemistry may be found elsewhere [24].

The EMST Mixing Model

The EMST model has the unique advantage of adequately representing the mixing of reactive and conserved scalars. At a given time, and within a given grid cell, a new "tree" is formed to account for the mixing that occurs between the particles in the cell. With σ being the number of compositions considered and N the number of particles in the cell, the composition of the ith particle ($i = 1, \ldots, N$) is denoted by $\phi^{\beta}_{(i)}$, $\beta = 1, \ldots, \sigma$. The particle compositions evolve by interactions with "neighbor" particles, which are defined by the EMST according to their proximity in composition space. A "tree" is formed with a set of edges (unordered pair of points defining a particle and its neighbor) connecting all particles such that the total length of edges is minimized. If the number of edges incident on the ith particle is denoted E_i, then the scalar properties of particles, $\phi^{\beta}_{(i)}$, evolve according to the following equation:

$$w_{(i)} \frac{d\phi^{\beta}_{(i)}}{dt} = -\alpha \sum_{v=1}^{E_i} B_v(\phi^{\beta}_{(i)} - \phi^{\beta}_{(i_v)}) \qquad (1)$$

where i_v represents the ith particle's neighbor in the vth edge. This is illustrated in Fig. 2, which shows a typical EMST formed in two-dimensional composition space using 800 stochastic particles. The model parameter α controls the rate of variance decay of the scalars. The numerical weight of the particle is denoted by $w_{(i)}$, and the model coefficients B_v associated with the edges determine the evolution of the scalar PDF with time. One disadvantage of the EMST is that its computational cost scales as N^2. Details about the model and its performance characteristics in a number of test conditions are given elsewhere [17].

Results and Discussion

All computations are performed for the following conditions: bulk jet velocity, $\bar{u}_j = 41$ m/s, burned pilot velocity, $\bar{u}_{pb} = 24$ m/s, co-flow air velocity, $\bar{u}_a = 15$ m/s. The initial conditions for the velocity and turbulence profiles are identical to those specified earlier for similar jet flames [5]. The mixture fraction at the jet exit plane in the jet, pilot, and air streams is 1, ξ_s, and 0, respectively. The solution grid covers the region from $x/D = 0$–25 and $r/D = 0$–10, where D is the fuel jet diameter ($D = 7.2$ mm). This is considered adequate since the region of interest is

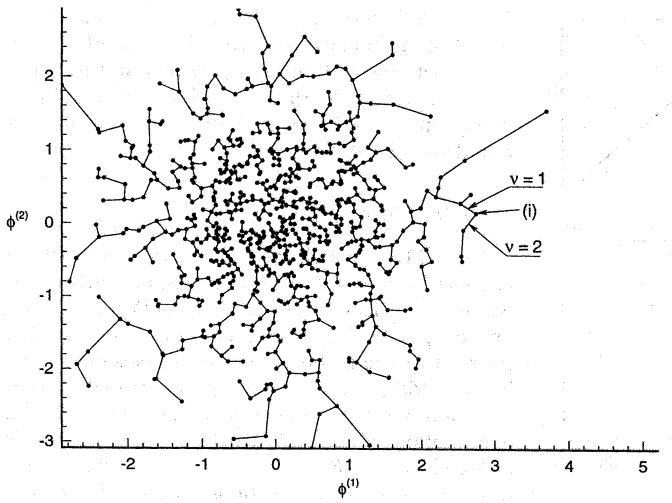

FIG. 2. The EMST formed from 800 particles in a two-dimensional composition space, showing the general particle i that in this case has two edges $v = 1$ and $v = 2$.

TABLE 1
Stoichiometric mixture fraction, ξ_s, X–Y grid size, lean and rich reactive limits, ξ_L and ξ_R, for the flames for which PDF simulations are performed

ξ_s	ξ_L	ξ_R	X–Y Nodes
0.055	0.045	0.185	31 × 21
0.305	0.225	0.495	31 × 21
0.5	0.305	0.695	31 × 21

centered just downstream of the pilot flame "shroud" that generally extends for a few jet diameters. (Before it is completely mixed, the pilot flame provides a shroud in the sense that it physically separates the fuel stream from the airstream.)

Numerical tests were performed to determine the choice of numerical parameters that minimize the computational cost of obtaining converged solutions that are reasonably independent of the grid size and the number of stochastic particles. At each time step, computations are carried out for all the particles in the solution domain. The time step is chosen to be the shortest of the convective, mixing, and reactive timescales. This ensures that these processes are resolved properly. It should be noted that using the same time increment for velocity and scalar mixing is justified for this type of shear flows because of the multistream geometry with different velocities and compositions. The solution is carried out over a long enough time to ensure convergence. With the EMST model, both mixing and reaction are performed simultaneously. This is a considerable advantage over previous approaches where these processes are computed separately.

Computations are performed for the same flame using three different grid sizes with X–Y nodes: 31 × 21, 46 × 31, and 61 × 41. This corresponds to 600, 1250, and 2400 cells, respectively, with 100 particles in each cell. The computed mean axial velocity, $\tilde{u}$, and mean mixture fraction, $\tilde{\xi}$, have been compared for the three grid sizes, and the 31 × 21 grid is found to be adequate. Computations with the EMST mixing model take about 2.5 times the CPU time required for a similar calculation using the IEM mixing model. Simulations performed with double the number of particles revealed little difference. The 31 × 21 grid with 100 particles per cell is, therefore, used in all further computations that are performed for three different stoichiometries with the conditions shown in Table 1.

Measurements of the velocity, turbulence, and mixing fields are available only for a piloted flame of methane fuel with $\xi_s = 0.055$. Computations are performed for a flame with the same stoichiometry and the results are then compared with the measurements (not shown here). The agreement is found to be adequate, considering the difference between the simple chemistry used here and that of methane fuel.

Figures 3 and 4 show computed scatter plots of progress variable b versus mixture fraction for two flames with $\xi_s = 0.305$ and 0.5, respectively. The computations are repeated using the IEM and EMST mixing models, and the results are shown in Figs. 3 and 4 for the ranges of x/D = 0–5, 5–15, and 15–25 of the solution domain. The first range from x/D = 0–5 corresponds to the region where the pilot shroud is still separating the fuel from the airstream and is shown in Figs. 3a and 4a. In this range, mixing mainly occurs between the pilot gases and either air or pure fuel. Originally, fluid particles issuing from the pilot stream with composition ($\xi = \xi_s, b = 1$), mix either with air ($\xi = 0, b = 0$) or with fuel (ξ

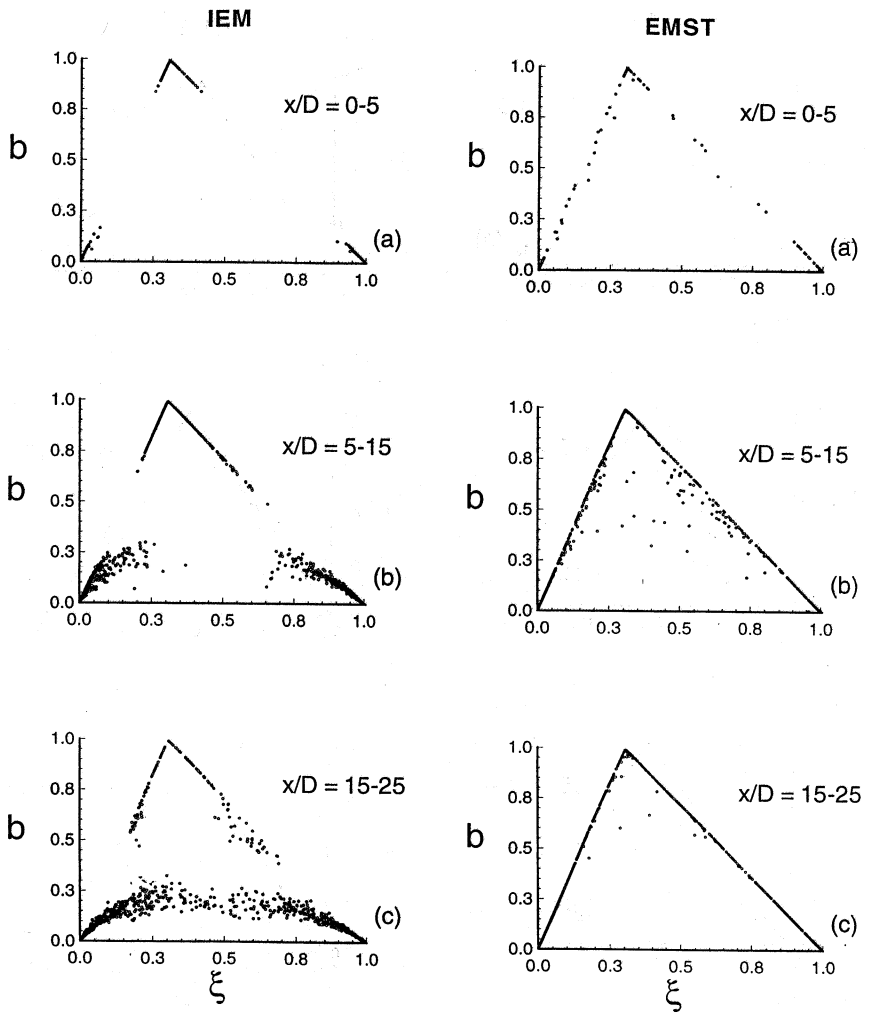

FIG. 3. Computed scatter plots of progress variable b versus mixture fraction ξ for the flame with $\xi_s = 0.305$ using the IEM and EMST mixing models. Each plot covers a specific axial range extending from (a) $x/D = 0$–5; (b) $x/D = 5$–15; (c) $x/D = 15$–25.

$= 1, b = 0$). Resulting particles populate the composition space that joins the following vertices: ($\xi = \xi_s, b = 1$), ($\xi = 0, b = 0$), ($\xi = 1, b = 0$). Figures 3 and 4 show that both the IEM and EMST models give comparable results in this region of the flow. This is expected considering that mixing is done mainly in one-dimensional scalar space where both models perform adequately.

Further downstream of the pilot flame shroud, fluid particles that originated from the pilot, air, and fuel streams may coexist in the same cell and are therefore likely to mix. It is in these regions of the flows that the mixing models are put to the test since two-dimensional mixing is more likely between particles with a range of conserved and reactive scalars. Figures 3b and 4b show a comparison between the IEM and EMST models for flame with $\xi_s = 0.305$ and 0.5 in the range $x/D = 5$–15. It is clear that the compositions resulting from the IEM model deviate from the fully burned compositions and start to populate the intermediate region. Fully burned compositions are those that lie on the line extending from ($\xi = 0, b = 0$) to ($\xi = \xi_s, b = 1$) to ($\xi = 1, b = 0$). The EMST model results in compositions that remain on the fully burned line regardless of the axial location. It should be noted that identical conditions are used for both the IEM and EMST simulations. The same trend continues further downstream as is shown in Figs. 3c and 4c for the range $x/D = 15$–25. It is also clear that these results

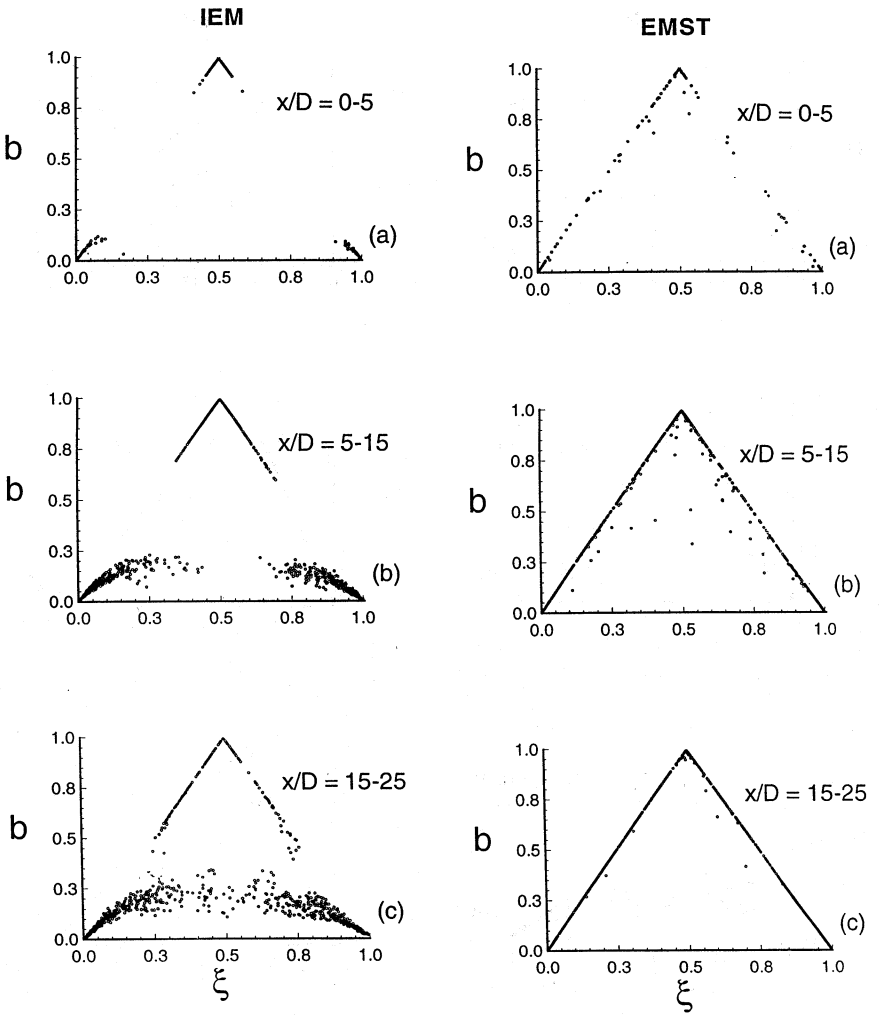

FIG. 4. Computed scatter plots of progress variable b versus mixture fraction ξ for the flame with $\xi_s = 0.5$ using the IEM and EMST mixing models. Each plot covers a specific axial range extending from: (a) $x/D = 0$–5; (b) $x/D = 5$–15; (c) $x/D = 15$–25.

are independent of the stoichiometry of the fuel mixture.

To validate these computations, joint imaging of temperature and mixture fraction has been performed in a pilot-stabilized flame of $H_2/N_2 = 1/1$ (by vol.). The fuel mixture has a stoichiometric mixture fraction of 0.305 and the chemistry is relatively fast. Temperature here may be thought of as a progress variable (b) with a value of 1 when the temperature corresponds to that of fully reacted fluid and a value of 0 when the temperature is that of unreacted fluid at 300 K. Contour plots representing the joint PDF of measured temperature and mixture fraction are shown in Fig. 5 for the a range of axial locations in the H_2/N_2 flame. These measurements should be compared with simulations for the flame with $\xi_s = 0.305$ shown in Figs. 3a and 3b for similar axial locations. It is evident from these plots that the EMST mixing model is showing the correct trend of mixing as opposed to the IEM model, which fills up the entire domain within the fully reactive and frozen limits. Although measurements do not extend further downstream, the trend is expected to be the same since the flames studied here are very far from blow off. It should be noted here that the pilot in the H_2/N_2 flame is shorter than that of the computed flame and extends for only about 3 jet diameters.

The IEM model mixes particles that may be well apart in composition space as long as these particles are in the same cell. This implies that particles with

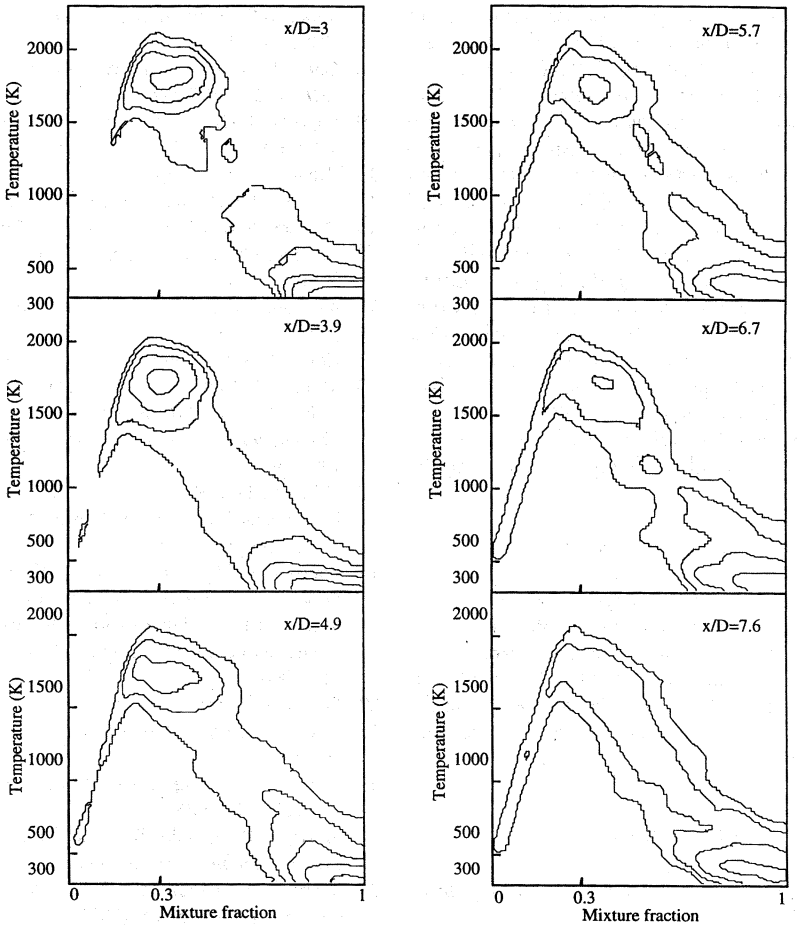

FIG. 5. Contours of the joint PDF of temperature and mixture fraction imaged at various axial locations in a jet flame of H_2/N_2 fuel with $\xi_s = 0.305$. Each image covers a range of 12 mm (1.6 diameters), and the axial location quoted on each plot corresponds to the center of the image.

compositions, say ($\xi = 0.75$, $b = 0.50$) and ($\xi = 0.15$, $b = 0.25$) may mix, leading to intermediate compositions that are well away from the fully burned line. With the EMST model, these particles will not mix together but will mix with others that are closer in composition space. It should be noted here that in the hypothetical case of very fast chemistry and very broad reactive limits, particles will be pushed immediately to the fully burned limit because of the fast reactions and the results will be similar regardless of the mixing model. On the other extreme, when three-scalar mixing occurs without reaction, the IEM and EMST models will give different results, especially in the region close to the jet exit plane. This forms an interesting test case that could be used to further validate these mixing models. Imaging experiments applied to a nonreacting, three-stream/three-scalar mixing test case will be very useful in revealing the mixing pattern and further validating the multiscalar mixing aspect of the model.

(Previously, Norris and Pope [21] applied PDF methods using the IEM mixing model to pilot-stabilized jet flames close to extinction. In view of the current findings, it is somewhat surprising that their results compare favorably with the experimental data. Although they used a different PDF model and different thermochemistry, it is not clear which specific difference is responsible for the different behavior observed.)

Conclusions

A new code that uses a particle–mesh method to solve the transport equation for the joint PDF of velocity composition and turbulent frequency has been used with a new mixing model based on EMST

and simple, one-step thermochemistry. Comparison with experimental measurements in pilot-stabilized flames demonstrate that the EMST successfully models multiscalar mixing, and, in particular, it overcomes serious defects in IEM and Curl's models arising from their violation of the localness principle.

The success of the EMST model marks a significant advance in the modeling of turbulent combustion with PDF methods. It is well-known that the weak link in this approach lies in the modeling of mixing, and success in this regard brings us closer to the goal of the accurate simulation of complex turbulent reacting flows with detailed chemical kinetics. The extensive computational requirement, however, remains a drawback that is addressed elsewhere [25]. Bluff-body stabilized flames and lifted flames are two cases in which the PDF approach incorporating the EMST mixing model is likely to make a significant impact.

Acknowledgments

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COMMENTS

J.-Y. Chen, University of California–Berkeley, USA. Have the authors carried out PDF simulation using modified Curl's mixing which is inexpensive relative to EMST?

Author's Reply. Not in this work, but in an earlier study [1], both Curl's model and the modified Curl model were applied to a zero-dimensional nonpremixed test case. As here, in that study it was demonstrated that these non-local models yield qualitatively incorrect behavior in the fast-chemistry limit.

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Norberto Fueyo, University of Zaragoza–LITEC, Spain. My impression is that you are using a rather coarse mesh. For the flames you have simulated, our experience is that, for coarse meshes, the flame does tend to be extinguished, regardless of the mixing model (or even the chemistry model) that one uses. Once the mesh is adequately refined

and a grid-independent solution reached, the problem disappears and then the flame does burn. Have you tested your computations for mesh independence?

Your mixing model seems to do a good job at keeping the reaction going; how does it perform when it comes to predicting extinction?

Author's Reply. We do not agree that extinction here is due to the coarse mesh rather than the mixing model. For the IEM mixing model, the grid was refined from 31 × 21 to 91 × 61 and the flame remained extinguished resulting in the same scatter plots as shown in Figs. 3 and 4 of the paper.

The EMST does indeed give a good representation of the mixing and hence it sustains reaction as illustrated in the paper using relatively fast and simple thermochemistry. Predicting extinction requires the implementation of realistic chemistry into the code. This is currently being done and, in conjunction with the EMST, it is expected to give good results.