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 tree (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 H2/N2 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 multiscale 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 [8] 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 multiscale 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

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 stochas-
mixing model for pdf simulations

2.0 \times 10^{-6} and \Delta x = 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 \sigma being the number of compositions considered and i the number of particles in the cell, the composition of the i-th particle (i = 1, ..., N) is denoted by \phi_{hi}, \beta = 1, ..., \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 i-th particle is denoted \hat{E}_i, then the scalar properties of particles, \phi_{hi}, evolve according to the following equation:

\omega_{hi} \frac{d\phi_{hi}}{dt} = -\alpha \sum_{i=1}^{\hat{E}_i} B_{ij} (\phi_{hi} - \phi_{hj}) \quad (1)

where \hat{i} represents the i-th particle's neighbor in the \hat{j}th 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 \alpha controls the rate of variance decay of the scalars. The numerical weight of the particle is denoted by \omega_{hi}, and the model coefficients B_{ij} 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, \nu = 41 m/s, burned pilot velocity, \nu_{pb} = 24 m/s, co-flow air velocity, \nu = 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, \xi, 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
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 time scales. 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 flow 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: \( 31 \times 21, 46 \times 31, \) and \( 61 \times 41 \). This corresponds to 600, 1250, and 2400 cells, respectively, with 100 particles in each cell. The computed mean axial velocity, \( \bar{u} \), and mean mixture fraction, \( \xi \), have been compared for the three grid sizes, and the \( 31 \times 21 \) 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 \( 31 \times 21 \) 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 \( \xi = 0.055 \). 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 \( \xi = 0.305 \) 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 \( (\xi = \xi_0, b = 1) \), mix either with air \( (\xi = 0, b = 0) \) or with fuel \( (\xi \)}
Fig. 3. Computed scatter plots of progress variable $b$ versus mixture fraction $\xi$ for the flame with $\xi_i = 0.305$ 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: $(\xi = \xi_i, b = 1), (\xi = 0, b = 0), (\xi = 1, b = 0)$. 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 $\xi_i = 0.305$ 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 $(\xi = \xi_i, b = 1)$ 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
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 \( \text{H}_2/\text{N}_2 = 1/1 \) (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 range of axial locations in the \( \text{H}_2/\text{N}_2 \) flame. These measurements should be compared with simulations for the flame with \( \zeta_r = 0.305 \) shown in Figs. 3a and 2b 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 \( \text{H}_2/\text{N}_2 \) 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
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 demonstrates that the EMST successfully models multiscale mixing, and, in particular, it overcomes serious defects in IEM and Curt’s models arising from their violation of the locality 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. 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.

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REFERENCES


COMMENTS

J.-Y. Chen, University of California–Berkeley, USA.

Have the authors carried out PDF simulation using modified Curt’s mixing which is inexpensive relative to EMST?

Author’s Reply. No. In this work, but in an earlier study [1], both Curt’s model and the modified Curt model were applied to a zero-dimensional nonpremixed test case. As here, in that study it was demonstrated that these nonlocal models yield qualitatively incorrect behavior in the fast-chemistry limit.

REFERENCE


Norberto Fuego, 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 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 31 × 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.