UC Berkeley
Combustion Modelling

Title

LES of Sandia Flame D with Eulerian PDF and Finite-Rate Chemistry

Permalink
https://escholarship.org/uc/item/8xf9z5wn

Authors

Bisetti, Fabrizio
Chen, J Y

Publication Date

2005-10-17

Peer reviewed

eScholarship.org Powered by the California Digital Library
University of California

LES of Sandia Flame D with Eulerian PDF and Finite-Rate Chemistry

Western States Section/Combustion Institute
2005 Fall Meeting
Stanford University, October 17-18, 2005

Paper number: 05F-33

Fabrizio Bisetti*
University of California, Berkeley
Jyh-Yuan Chen
University of California, Berkeley

* Corresponding author: fbisetti@me.berkeley.edu

LES of Sandia Flame D with Eulerian PDF and Finite-Rate Chemistry

Fabrizio Bisetti [*], J.-Y. Chen

Department of Mechanical Engineering, University of California at Berkeley, 94720 Berkeley, CA USA

Abstract

Monte Carlo simulations of joint PDF approaches have been extensively developed in the past largely with Reynolds Averaged Navier Stokes (RANS) equations. Current interests are in the extension of PDF approaches to Large Eddy Simulation (LES). As LES allows to resolve the large scales of turbulence in time and space, a joint LES-PDF approach holds the promise to ease the modelling requirements (e.g. mixing models). In the past we have implemented a joint scalar PDF approach into LES with the flamelet model using an Eulerian approach. Our preliminary results demonstrated that careful implementation of the Eulerian approach can be fully consistent with the counterpart finite-volume method. In this paper, results of recent LES of a pilot CH_4/Air flame (Sandia/TUD flame D) with realistic finite-rate chemistry will be reported using three different mixing models including modified Curl (MC), Interaction by Exchange with the Mean (IEM), and Eucledian Minimum Spanning Tree (EMST). The calculations were performed with a 12-step reduced chemistry that has been well tested in RANS simulations of Sandia Flame D. In constrast to established RANS results which showed unphysical extinction with selected mixing models, LES results with different mixing models all lead to stable combustion and somewhat similar extinction patterns. These results suggest that the requirements of mixing models may be relaxed if large variations in scalar composition are coherently resolved as shown by our implementation of a joint LES-Eulerian PDF approach.

Key words: Turbulent combustion, Eulerian PDF methods, Mixing models, Large Eddy Simulation;

---

1. Introduction

Current interest is in the application of Probability Density Function (PDF) methods to Large Eddy Simulation (LES). As noted recently by Bilger et al. (2005), the framework of LES alleviates the demands on the micromixing (molecular mixing) models, as a larger portion of sub-grid scale fluctuations is resolved (as opposed to RANS). Additionally, LES arguably enforces a higher degree of locality in composition space, as it resolves finer structures. Finally, LES provides more information to be used in the mixing models (Bilger et al., 2005). Sub-grid scale mixing is a key process in the behavior of non-premixed turbulent combustion systems close to states relevant to engineering applications, such as ignition, extinction, and possibly reignition. While it is a well accepted paradigm of turbulent combustion that extinction and reignition are governed by the interaction between chemistry and the local (high) gradients in the scalar fields, the actual inner dynamics of the process are just starting to be exposed (Hult et al., 2000). Past experience with turbulent non-premixed flames PDF computations (Tang et al., 2000; Xu and Pope, 2000; Lindstedt et al., 2000) proved the ability of PDF methods to capture extinction in a variety of flames. Nevertheless, the actual coupling between the choice of mixing models and the ability of capturing the extinction process is yet to be fully uncovered. It is safe to expect that different mixing models will predict

---

[*] Corresponding author: fbisetti@me.berkeley.edu

different degrees of extinction, but quantitative studies in the context of LES have only started recently, and more work is needed as expressed in the last two most recent workshops on Turbulent Nonpremixed Flames (TNF, 2002, 2004). Very recently, Mitarai et al. (2005) have performed an extensive study on the performance of mixing models in the framework of RANS, and LES, by successive filtering of Direct Numerical Simulation data for non-premixed turbulent flames undergoing extinction and reignition. Their study (Mitarai et al., 2005) shows that transitioning from RANS to LES, the mixing models perform more similarly one to the other, thus confirming the intuition about the merit of LES in reducing the scale gap, so that modeling requirements are eased. Additionally, attempts to quantify the differences and similarities of the available mixing models in a more fundamental way are still underway. Ren and Pope (2004) performed a controlled comparison (Partially Stirred Reactor) of Interaction by Exchange with the Mean (IEM/LMSE) model (Dopazo and O'Brien, 1974), modified Curl (MC) model (Janicka et al., 1977), and Euclidean Minimum Spanning Tree (EMST) model (Subramaniam and Pope, 1998). Recently, the authors of the present paper reported preliminary findings of an investigation regarding the basic requirements for a seemless integration of an Eulerian PDF method into an incompressible LES (Bisetti and Chen, 2005). In particular, we devised a methodology to assure that the mean of the mixture fraction PDF (ensemble average) matches instantaneously and locally the mixture fraction redundantly computed from the LES finite volume scheme, so to harness coherently all the available information from the flow field computed by the LES. In the present paper we report the results of recent LES of Sandia Flame D with an Eulerian PDF approach and realistic finite-rate chemistry. The goal set forth by our computations is two-fold. On one hand we compare the performance of the three main mixing models (IEM, MC, and EMST) in the framework of LES of piloted CH_4/Air flames (Barlow and Frank, 1998). On the other hand, we test the overall predicting abilities of our novel fully coherent Eulerian PDF method, which we recently extended to second order accurate in space and third order accurate in time. Data reduction similar to Xu and Pope (2000) is adopted in order to stress the extinction predictions, as compared to experimental data from Barlow (2003).

2. Formulation of the problem and solution method

A cylindrical mesh is used to cover the computational domain from the jet inlet up to $x/D = 20$. The mesh extends from the centerline to $r/D = 10$ in the radial direction for the entire axial length. Due to stringent constraints to the computational resources available to the authors, the mesh is admittedly coarse with 250 equally spaced nodes in the direction of the jet axis, 32 equally spaced azimuthal, and 37 nodes along the radial direction (clustered towards the centerline). A mesh convergence study based on a parallel version of the same code here used is scheduled for the near future. The flow field is solved with an incompressible predictor-corrector TVD scheme, which is second order in space. The time integration is performed explicitly with a compact Runge Kutta third order scheme. The well established adaptive filtering technique by Germano et al. (1981) is used to obtain the eddy viscosity. Additionally, the chemistry is integrated via In Situ Adaptive Tabulation (ISAT) as developed by Chen (2004). The kinetics are computed given a reduced mechanism comprising 16 species and 12 reactions (Chen, 1999). The stoichiometric composition is $F_s = 0.351$ (Barlow, 2003). The turbulent (filtered) inlet boundary conditions for the main stream and the coflow are generated using the technique outlined in Klein et al. (2003).

2.1. *Eulerian PDF methodology*

We let the probability density function $P_\Phi(\phi; \mathbf{x}, t)$ describe the probability density for the occurrence of a given set of scalars at prescribed location and time. We adopt a Monte Carlo method for the solution of the PDF transport equation as in Pope (1981). The present PDF calculations are not coupled with the flow field, i.e. the local properties are calculated using a flamelet approach, and not the local, instantaneous PDF solution. As a result, all mixing models experience an identical flow field. The treatment of the convective fluxes is of order higher than one, and fully consistent with the solution from the second order finite volume scheme. This implies that at every instant t, and every location $\mathbf{x}$, the ensemble average of the mixture fraction from the PDF transport solution is identical to the LES resolved value of the conserved scalar. The subscale fluctuations (i.e. fluctuations occurring on a scale smaller that the scales resolved by the LES) are resolved by the notional particles population. Due to the limited computational resources available to the authors for the present computations, only 20 particles on each node have been employed and no further stochastic convergence study could be performed. Operator splitting is used to advance the PDF in time by evolving P_Φ due to *(i)* convection (resolved and modeled sub-grid-scale velocities) in physical space, *(ii)* micromixing (via mixing models) and *(iii)* reactions (via ISAT) in scalar space.

3. Statistics

Statistics are collected after several flow residence times have passed from the onset of the computation. A residence time is estimated from the flight time (domain length divided by bulk velocity) as 2.8 ms. In order to compare our results to the available experimental data (Barlow, 2003), we collected particles on the $x/D = 15$ plane at different radial locations, coherently with experimental practice. Following the reccomendations from past TNF workshops we report results on radial statistics, scatter plots and conditional statistics and PDF. We focus our attention on temperature, mixture fraction, and CO mass fraction data.

3.1. *Radial profiles*

The radial profiles for temperature and mixture fraction are presented in Figures 1(a)-(d). Note that the average (filtered and ensemble from PDF) for the conserved scalar as in Figure 1(c) is identical for all of the mixing models, as expected, given the uncoupled nature of the simulation (see Section 2.1), which excludes feedback from the PDF solution to the flow solver. Overall, the qualitative agreement with the experimental data is encouraging. Also, all mixing models produce very similar results, as it might be expected when the amount of unresolved fluctuations decreases transitioning from RANS to LES. Additionally, it is interesting to compare the somewhat homogeneous behavior of the solution across mixing models to the occurrence of unphysical flame blow-out observed in some RANS computations with IEM mixing model (TNF, 1998). The average temperature is well within 20% at the location of largest error. On the other hand, mixture fraction is within 30%, where the error is the largest. The total fluctuations (resolved by LES and subgrid PDF fluctuations) are captured correctly for the mixture fraction, while large errors seem to be present for temperature. In both cases, the general trend is correctly predicted.

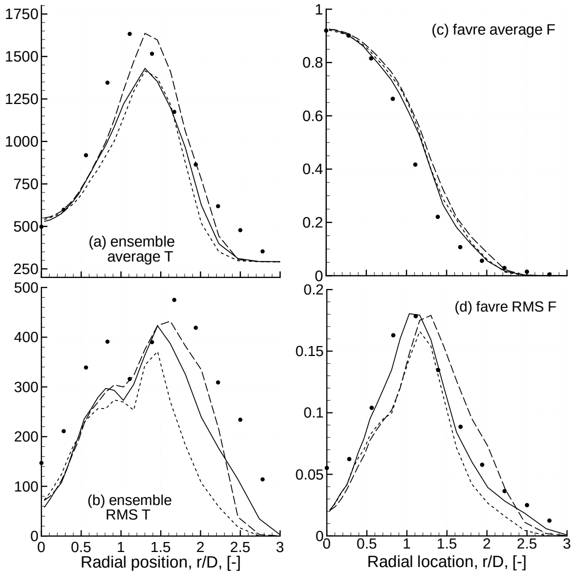

Fig. 1. Mean and RMS for temperature (left, a-b) and favre average and RMS of mixture fraction (right, c-d) along the radial direction at $x/D = 15$ from experiments (symbols) (Barlow, 2003), and from LES using IEM (solid), MC (dashes), and EMST (long-dashes) mixing models.

3.2. *Scatter plots*

Scatter plots show a qualitative agreement of temperature (Figure 2) and CO mass fraction (Figure 3) samples at $x/D = 15$ between all models and the experimental data. The data also compare well with the results presented in the last TNF workshop (TNF, 2004). In particular, all models yield a steadily burning solution. Of all the models, EMST seems to be the one that captures best the temperature. On the other hand, as reported by other authors (Ren and Pope, 2004) we find IEM and MC models to predict too many samples at low temperatures, hence resulting in excessive extinction occurrence. Yet, the behavior across models is quite similar, and it might be argued whether or not the observed differences are within numerical error. The predicting abilities of EMST seem to deteriorate as far as Y_{CO} scatter plots are concerned, where MC seems to perform better.

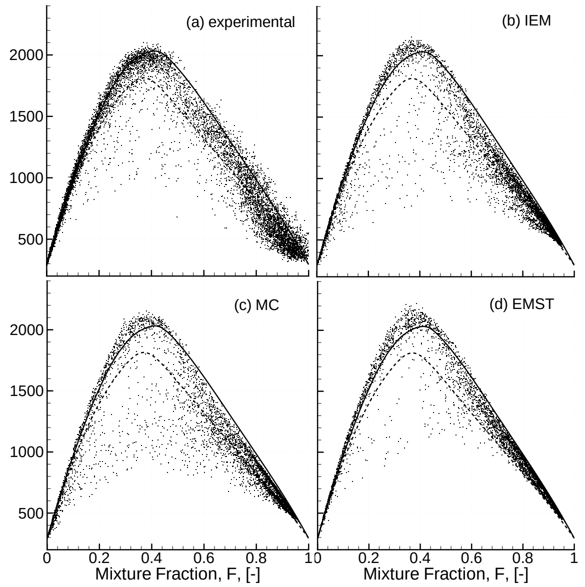

Fig. 2. Scatter plots of temperature versus mixture fraction using some 10k samples at $x/D = 15$ from *(a)* experimental data (Barlow, 2003), and from LES using *(b)* IEM, *(c)* MC, and *(d)* EMST mixing models.

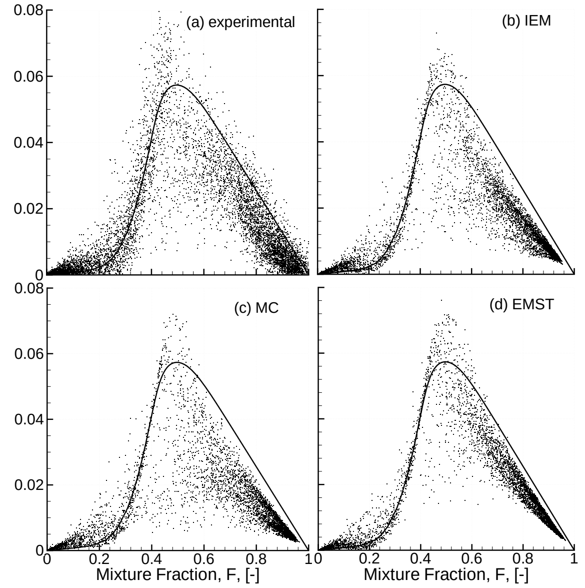

Fig. 3. Scatter plots of CO mass fraction versus mixture fraction using some 10k samples at $x/D = 15$ from *(a)* experimental data (Barlow, 2003), and from LES using *(b)* IEM, *(c)* MC, and *(d)* EMST mixing models.

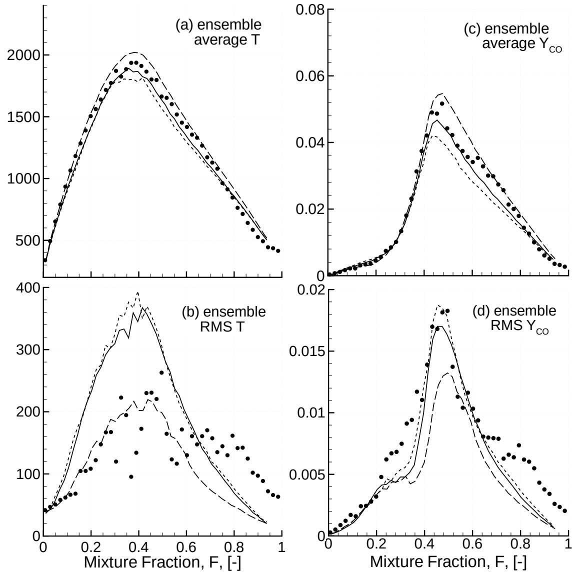

Fig. 4. Averages and RMS (ensemble) of the CPDF (Conditional PDF) of T (left, a-b) and CO mass fraction (right, c-d) at $x/D = 15$ from experiments (symbols) (Barlow, 2003), and from LES using IEM (solid), MC (dashes), and EMST (long-dashes) mixing models.

3.3. *Conditional plots*

Upon conditioning on the mixture fraction we are able to present statistics and actual PDF of relevant scalars (T and Y_{CO}) versus the conditioning variable F. Again, the models perform similarly. Averages are extremely close one to the other and to the experiemental data, while fluctuations do show differences. In particular, EMST is able to capture the range of temperature fluctuations much more accurately than the other models, which, by overpredicting the spread in temperature, are also more prone to extinction. On the other hand, the predictions for the fluctuations in Y_{CO} are poor, and MC and IEM perform better. Upon inspection of the CPDF of temperature (see Figs. 5(a)-(c)), it becomes clear that the PDF shapes produced by MC and IEM present a slight bi-modal nature (peaks centered at around 1000 K and 2200 K) that increases the spread and indicates extinction. The experimental data do present some extinction, but to a much lower extent. The results from EMST show less extinction, as the extinguished mode is less probable than in the IEM and MC calculations. Additionally, all computations seem to slightly overpredict the most probable temperature. The shape and quantitative features of the CPDF for CO mass fraction are captured more accurately by IEM and MC, while, as expected from the scatter plots, EMST's results are less accurate, in particular, the spread is underpredicted. Nevertheless, the results are overall encouraging.

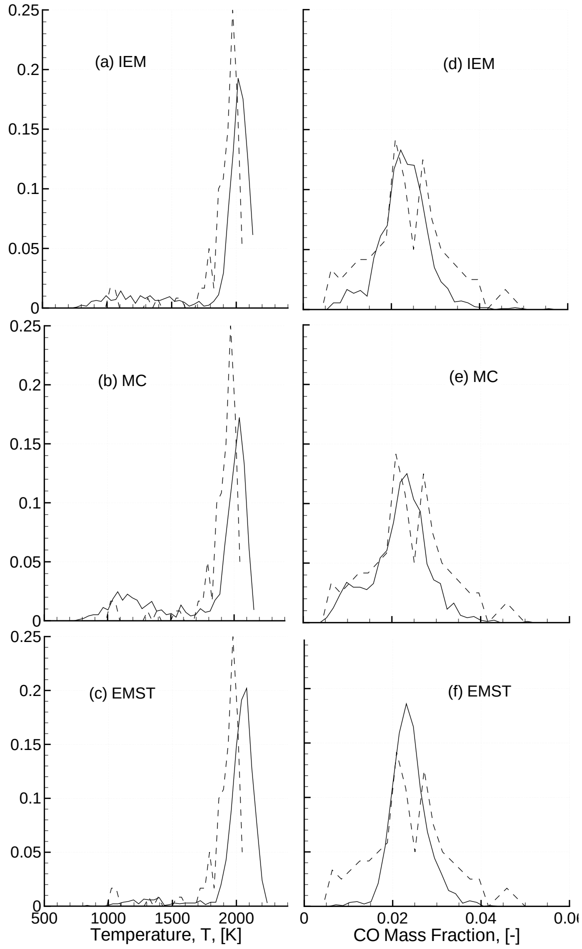

Fig. 5. Conditional Probability Density Functions (CDF) for $0.34 < F < 0.36$ at $x/D = 15$ for experimental and LES data of T (left, a-b-c) and CO mass fraction (right, d-e-f). On each plot we compare the experimental data (dashes) (Barlow, 2003) with the results from a different mixing model (solid).

3.4. *Analysis of extinction patterns*

In order to asses qualitatively the resilience to extinction of the different mixing models we processed scatter plots (single time measurements) of temperature versus mixture fraction (see Figure 2). By classifying an extinction event if the temperature at the given mixture fraction is lower than the temperature of the last burning flamelet near extinction, we were able to categorize the scatter data as either burning or not burning. Later we reduced the classification to a probability of extinction conditioned on the mixture fraction. The results are shown in Fig. 6 were we compare the different mixing models to the experiemental data. It is apparent that all mixing models predict a low probability of extinction near stoichiometric composition. Also, all models produce a steadily burning solution. Nevertheless, the extinction patterns are different. As shown by Ren and Pope (2004) and by Mitarai et al. (2005), we also find the EMST model to be produce less extinction, as it should naturally result from the enforcement of locality in composition space, which prevents 'hot' and 'cold' particles from mixing. As a result of the model inducing resistance to extinction, the mean conditional temperatures are higher and conditional variance in temperature are lower for EMST compared to other models. All models cannot capture the behavior on the rich side. Nevertheless, the merit of such comparison at rich compositions is questionable, as experimental data might be unconclusive near F=1. Yet, it seems clear that while IEM and MC show a minimum in the extinction probability near stoichiometric, whereas EMST shows no such minimum. To conclude, the prediction by EMST is quite accurate near stoichiometric, but the overall trend still remains almost completely unpredicted.

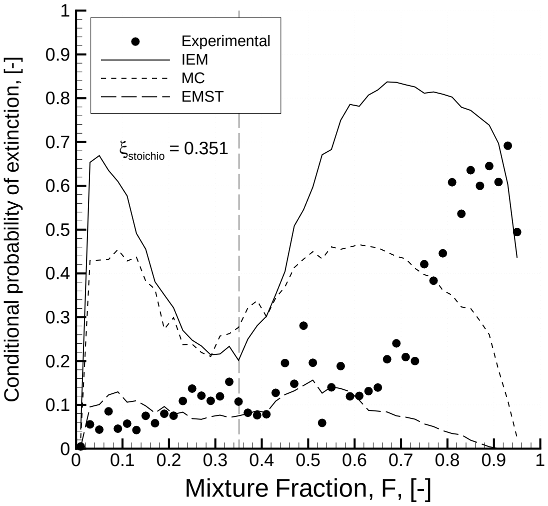

Fig. 6. Probability of extinction conditioned on the mixture fraction at $x/D = 15$. The data is obtained definining an extinction event if the temperature at a given mixture fraction lies below the last burning flame as from Tsuji burner calculations. Note that all mixing models overpredict the occurrence of extinction, with the exception EMST mixing model.

4. Conclusions

Extinction in turbulent flames is an extremely important, yet elusive process. The ability of predicting and eventually controlling extinction has a great practical value as far as the design of complex combustion systems is concerned. LES methods have imposed themeselves as the new stadard in turbulent computations, and their implementation in the existing framework of PDF methods for turbulent combustion has started. In this paper we reported some of the main results obtained from simulations of Sandia's piloted methane-air flame D with an Eulerian PDF method coupled to an incompressible LES. We used three different mixing models (IEM, MC, and EMST) and compared both general statistics and extinction predictions. We conclude that the results across mixing models are quite similar. Interestingly, all mixing models produce a burning solution, contrary to previous experience with RANS. We speculate that this behavior might be due to the ability of LES to resolve finer scales, thus easing the requirements placed on mixing models. In general, EMST model seems to perform better in predicting the temperature PDF conditioned on the mixture fraction. Also, the occurrence of extinction is nearly correctly predicted quantitatively near stoichiometric, but the overall trends are still erroneous. Amont all mixing models, EMST (C_Φ=2.0) allows obtaining the most accurate predictions on extinction likelihood near stoichiometric. Future work will concentrate on mesh refinement and particles refinement study.

References

Barlow, R. S., 2003. Sandia piloted CH_4/air flame D data - Release 2.0. `http://www.ca.sandia.gov/TNF`.

Barlow, R. S., Frank, S. A., 1998. Effects of turbulence on species mass fractions in methane-air jet flames. In: Proc. Combust. Inst. Vol. 27. pp. 1087–1095.

Bilger, R. W., Pope, S. B., Bray, K. N. C., Driscoll, J. F., 2005. Paradigms in turbulent combustion research. In: Proc. Combust. Inst. Vol. 30. pp. 21–42.

Bisetti, F., Chen, J.-Y., 2005. Numerical issues of Monte Carlo PDF for Large Eddy Simulation of turbulent flames. 4th Joint Meeting of the U.S. Sections of the Combustion Institute, Philadelphia (USA), March 20-23, 2005. Paper E28. Available at `http://repositories.cdlib.org/cpl/cm/BisettiJUSS05`.

Chen, J.-Y., 1999. Reduced mechanism for CH_4/air combustion (12-steps, 16-species). `http://www.ca.sandia.gov/TNF/chemistry.html`.

Chen, J.-Y., 2004. Analysis of In Situ Adaptive Tabulation performance for combustion chemistry and improvement with a modified search algorithm. Combust. Sci. and Tech. 176, 1153–1169.

Dopazo, C., O'Brien, E. E., 1974. An approach to the autoignition of a turbulent mixture. Combust. Sci. and Tech. 1, 1239–1266.

Germano, M., Piomelli, U., Moin, P., Cabot, W., 1981. A dynamic subgrid-scale eddy viscosity model. Combust. Sci. and Tech. 25, 159–174.

Hult, J., Josefsson, G., Aldén, M., Kaminski, C., 2000. Flame front tracking and simultaneous flow field vizualisation in turbulent combustion. In: Proceedings of the 10th International Symposium on Applications of Laser Techniques to Fluid Mechanics. Lisbon, July 10-13.

Janicka, J., Kolbe, W., Kollman, W., 1977. Closure of the transport equation for the PDF of turbulent scalar fields. J. Non-Equilib. Thermodyn. 4, 47–66.

Klein, M., Sadiki, A., Janicka, J., 2003. A digital filter based generation of inflow data for spatially developing direct numerical or large eddy simulations. J. Comput. Phys. 186 (2), 652–665.

Lindstedt, R. P., Louloudi, S. A., Vaos, E. M., 2000. Joint scalar probability density function modeling of pollutant formation in piloted turbulent jet diffusion flames with comprehensive chemistry. In: Proc. Combust. Inst. Vol. 28. pp. 149–156.

Mitarai, S., Riley, J. J., Kosály, G., 2005. Testing of mixing models for Monte Carlo probability density function simulations. Phys. Fluids 17.

Pope, S. B., 1981. A Monte Carlo Method for the PDF equations of turbulent reactive flow. Combust. Sci. and Tech. 25, 159–174.

Ren, Z., Pope, S. B., 2004. An investigation of the performance of turbulent mixing models. Combust. Flame 136, 208–216.

Subramaniam, S., Pope, S. B., 1998. A mixing model for turbulent reactive flows based on euclidean minimum spanning trees. Combust. Flame 115, 487–514.

Tang, Q., Xu, J., Pope, S. B., 2000. Pdf calculations of local extinction and no production in piloted-jet turbulent methane/air flames. In: Proc. Combust. Inst. Vol. 28. pp. 133–139.

TNF, 1998. Proceedings of the 3^{th} International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames. `http://www.ca.sandia.gov/TNF`.

TNF, 2002. Proceedings of the 6^{th} International Workshop on Measurement and Computation of

Turbulent Nonpremixed Flames. `http://www.ca.sandia.gov/TNF`.

TNF, 2004. Proceedings of the 7^{th} International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames. `http://www.ca.sandia.gov/TNF`.

Xu, J., Pope, S. B., 2000. Pdf calculations of turbulent nonpremixed flames with local extinction. Combust. Flame 123, 281–307.