

A constructed PDF model for fast CFD with realistic chemistry

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CFD predictions using a new model to include finite-rate chemistry effects in turbulent flames are presented. The Constructed PDF model assumes that the scalar PDF in a general, complex geometry reacting flow is similar to the scalar PDF in a simple geometry reacting flow. Detailed chemistry simulations are performed in a model of the simple flow over all realizable conditions. The scalar PDF at discrete points in the realizable space is parameterized by a small set of its lower moments, and tabulated. Modeled transport equations for these lower moments are computed in the CFD solver and the PDF table is interpolated for unclosed terms. *A priori* calculation and tabulation of the chemistry and its interaction with the turbulence allow rapid, multi-physics CFD simulations on large meshes. The model is applied to the RANS prediction of turbulent, partially-premixed, piloted jet flames (Sandia flames D and F). Excellent agreement with the experimental data is obtained for temperature, major species and the fast chemistry radical *OH*. Good agreement is obtained for *CO* and the slow chemistry species *NO*.

1. Introduction

Turbulent combustion models that incorporate arbitrary, detailed chemical kinetics in multi-dimensional CFD include the Transported PDF Model (Pope 1985), the Conditional Moment Closure (Klimenko & Bilger 1999) and the Steady and Unsteady Laminar Flamelet Models (Peters 2000). Owing to the tremendous computational cost of solving detailed chemical kinetics in complex three-dimensional geometries, combustion models that tabulate the chemistry and its interaction with the turbulence *a priori* remain prevalent in industry. The most common chemistry tabulation approach is the Steady Laminar Flamelet Model (SLFM) where a stationary flame is computed in a laminar flow configuration and mapped to a reduced variable space, usually mixture fraction and scalar dissipation rate or reaction progress variable. To account for turbulent fluctuations, a shape for the Probability Density Function (PDF) of these reduced variables is assumed, which is invariably a product of Delta functions (specified by first moments), and Beta or Gaussian functions (specified by first and second moments). The flamelet state relationships are convoluted with the assumed PDFs and tabulated as a function of the lower moments. Transport equations for these lower moments are solved in the CFD code, and the table interpolated to retrieve the required thermo-chemistry, such as mean density and mean temperature.

There are two limitations to the SLFM. The first is that the chemistry may be insufficiently represented by the reduced variables. For example, in the case of scalar dissipation rate as a flamelet reduced variable, the chemistry is assumed to respond instantaneously to the strain. This is a poor assumption for slow kinetics such as pollutant formation, which are predicted to be near equilibrium at the combustor outlet where the strain rate

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is small. The second limitation is that it is difficult to prescribe the joint PDF of the reduced variables, especially for those that are not conserved, and statistical independence of variables is invariably assumed.

The objective of this work is to apply the Constructed PDF Model (Goldin & Menon 1997; Goldin & Menon 1998; Goldin 2004) to an *a posteriori* CFD prediction of an experimental flame with comprehensive measurements, and to investigate its accuracy and performance. The Constructed PDF Model assumes that the thermo-chemical PDF in a turbulent reacting flow of arbitrary geometry is similar to the thermo-chemical PDF in a turbulent reacting flow of simple geometry. Reduced models for scalar evolution in simple geometric configurations are available, allowing affordable simulations with detailed chemistry over the entire range of realizable conditions. A suitable set of lower moments are selected to parameterize the PDF, and all required lower moments (such as mean density, mean temperature and if necessary mean reaction rate) are tabulated as a function of these lower moments. As in the SLFM, transport equations for the parameterizing lower moments are solved in the CFD code and all required PDF quantities are interpolated from the table. The Constructed PDF Model is directly comparable with the SLFM because they both pre-compute the turbulence-chemistry interaction and have similar storage and computational costs in the CFD solver. However, the Constructed PDF Model avoids the SLFM assumptions of state relationships and assumed PDF shapes.

2. The Constructed PDF Model

In this work, the joint PDF of species and temperature is constructed from scalar mixing and reaction in the simple geometry of isotropic, homogenous, stationary turbulence. Three dimensional Direct Numerical Simulations (DNS) with full chemistry at high Reynolds numbers is computationally impossible at present, so the Linear Eddy Model (LEM) (Kerstein 1988, Kerstein 1992) is employed to make the computations tractable. The LEM is an excellent approximation of scalar evolution in simple geometries, and accurate statistics of the scalar PDF in homogenous turbulence have been demonstrated (McMurtry *et al.* 1993).

The central assumption of the LEM is that since reaction occurs at the molecular level after species mix, it is critical to resolve the smallest turbulent length scales, which contribute substantially to mixing. Hence, mixing models, such as gradient-diffusion or coalescence-dispersion, are not invoked. To make such DNS affordable, the spatial dimension is reduced from 3D to 1D. Along a 1D line, molecular diffusion and chemical reaction are resolved without approximation, but turbulent convection by 3D eddies must be modeled. This stirring is modeled by random re-arrangements of the scalar elements along the LEM line, where each mapping imitates the effect of a turbulent eddy on the scalar field. The turbulence is hence specified in the LEM by two parameters, namely integral length scale L and Reynolds number Re_t (or equivalently the Kolmogorov length scale $\eta = L/Re_t^{3/4}$). Since the LEM is a Monte-Carlo simulation, statistics must be averaged over a number of realizations.

The LEM scalar field is smoothed by the continuous action of molecular diffusion and sharpened by irregular turbulent stirring events. For large L and small Re_t , the Kolmogorov scale is large and the flame chemistry is near equilibrium[†]. As Re_t increases,

[†] Slowly forming chemical species such as *NO* may be far from chemical equilibrium even at low Re_t .

smaller eddies appear and occur with increased frequency. They cause fine-scale gradients in the scalar field, increasing the rate of molecular diffusion and the degree of chemical non-equilibrium. At moderate Re_t local extinction occurs, and at high Re_t all flame structures in the LEM field blow-out. Although the LEM model has two turbulence inputs (viz. L and Re_t), the scalar PDF is not independent of these two parameters, and similar PDFs are obtained for different L and Re_t combinations (Goldin & Menon 1997). To illustrate this, note that the LEM domain length is equal to L , and the boundary conditions are periodic. Hence, a domain of size $2L$ with a larger Re_t so that both simulations have identical Kolomogorov length scales η will have identical PDFs.

With a specified mechanism and molecular transport properties, the two LEM inputs are the initial scalar field and the LEM turbulence parameters L and Re_t . By varying these two parameters over their realizable ranges, the joint PDF of species and temperature is tabulated as a function of a (small) set of its lower moments.

3. Constructing the PDF Table

The Constructed PDF Model is applied here to non-premixed combustion. Accordingly, the initial scalar field is a slab of fuel adjacent to a slab of oxidizer. A conserved mixture fraction can be defined from the LEM species field, and its Favre mean remains constant during the scalar field development. The mixture fraction variance decays monotonically from a maximum at the start of the simulation, toward zero. In this work, the scalar PDF is parameterized by these first two moments of the mixture fraction. An additional moment is required to parameterize the turbulence: simulations at low turbulence where the chemistry is near equilibrium will take longer to dissipate than high turbulence simulations, but will still pass through the same mixture fraction variance. Here, the mean scalar dissipation rate is used as a third parameter[†].

We apply the Constructed PDF Model to CFD predictions of the Sandia piloted jet flames labeled D and F. A well-validated, 19 species chemical mechanism for methane-air combustion is used (Sung *et al.* 2001) which is a CARM reduction from the GRI-Mech 2.11 detailed mechanism. ISAT (Pope 2001) is utilized to accelerate the chemistry calculations and radiative heat loss by an optically thin model is included (Barlow *et al.* 2001). Constant molecular transport properties are assumed, with a Schmidt number of 0.7 and a unity Lewis number. Since the initial condition is cold fuel next to cold oxidizer, ignition is necessary to initiate combustion. Ignition is modeled by equilibrating mixed-but-unburnt elements at early stages in the simulation. Note that the PDF at later times is relatively insensitive to this artifact (Goldin 2004).

The mean mixture fraction uniquely defines the initial scalar field and 16 points are used in mean mixture fraction space. At each mean mixture fraction, we fix L at 0.1m and run the LEM at 5 Re_t values of 100, 500, 1000, 1500 and 2000. The mixture fraction variance decays from its maximum to zero in every LEM simulation, and the PDF is tabulated at 24 intermediate variance points. All LEM simulations are ensemble averaged over 100 realizations to remove statistical errors. Approximately 1000 CPU hours are required to build this table.

RANS simulations of flames D and F are performed using this constructed PDF table. For isobaric combustion, the thermo-chemistry couples to the flow through the mean density which is obtained from the table by tri-linear interpolation. The $k-\epsilon$ turbulence

[†] Mean residence time and mean reaction progress were tested in place of mean scalar dissipation rate and found to be less accurate.

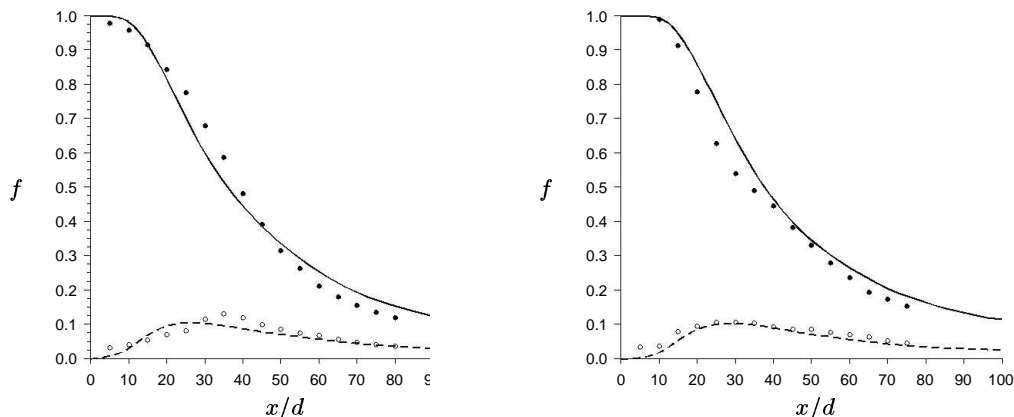


FIGURE 1. Axial plot of mean and RMS mixture fraction (f) for flame D (left) and flame F (right). Solid line is the predicted mean, solid circles are experimental mean, dashed line is the predicted RMS, open circles are experimental RMS

model is used with standard constants except for $c_{\epsilon 1}$, which is increased to 1.56 so that the correct jet spreading is obtained. Standard equations for mean and variance of mixture fraction are solved (Peters 2000), with the turbulent Schmidt number set to 1, and the standard model for the mean scalar dissipation rate is used, with $c_{\phi} = 2$. All RANS simulations are performed on an axi-symmetric mesh and take minutes to converge on a laptop computer.

4. Results

Axial plots of mean and RMS mixture fraction, temperature and OH , CO and NO mass fractions are presented in Figures 1 through 5. Plots on the left correspond to flame D and plots on the right to flame F. The predicted mean and RMS of mixture fraction in Figure 1 show reasonable agreement with the data. Since the mixture fraction is a conserved scalar, this difference is attributed, mostly, to deficiencies in the RANS turbulence model. Mean temperature prediction in Figure 2 show very good agreement for flame D, and moderate agreement for flame F. The Flame F experiment is near global blow-off and exhibits significant local extinction at all measured axial stations, which is difficult to predict. While the LEM is capable of predicting local extinction, parameterizing this by the single variable of mean scalar dissipation rate has limitations. The major species CH_4 , O_2 , CO_2 and H_2O show similar agreement as temperature and are excluded here.

Excellent agreement for mean and variance of OH mass fraction is displayed in Figure 3. In particular, the super-equilibrium increase of OH as the strain is increased from flame D (left) to flame F (right) is captured.

CO mass fraction in Figure 4 is reasonably well computed, but is over-predicted in the rich zones before the flame stoichiometric point at approximately $x/d = 45$. H_2 mass fraction displays similar behaviour as CO , hence plots of H_2 are not included here. In order to better understand the rich-side over-prediction of CO in Figure 4 conditional averages of CO are presented in Figure 5 for axial stations $x/d = 30$ and $x/d = 45$ in flame

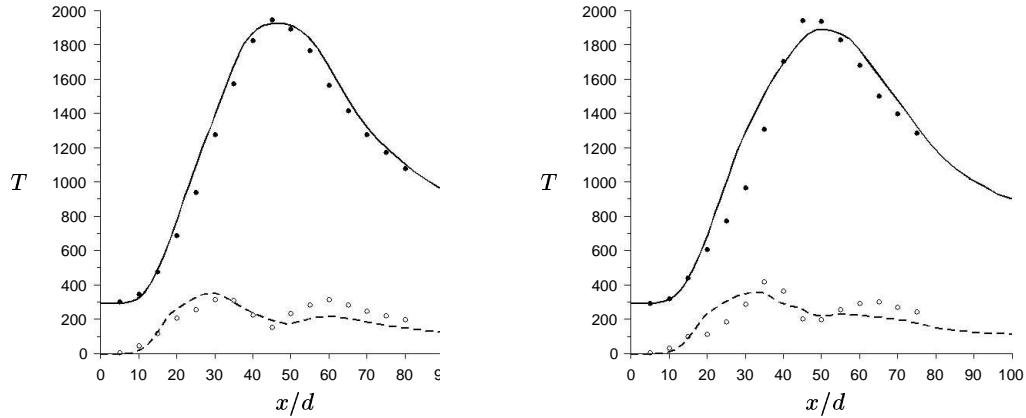


FIGURE 2. Axial plot of mean and RMS temperature (in degrees Kelvin) for flame D (left) and flame F (right). Symbols as in Figure 1.

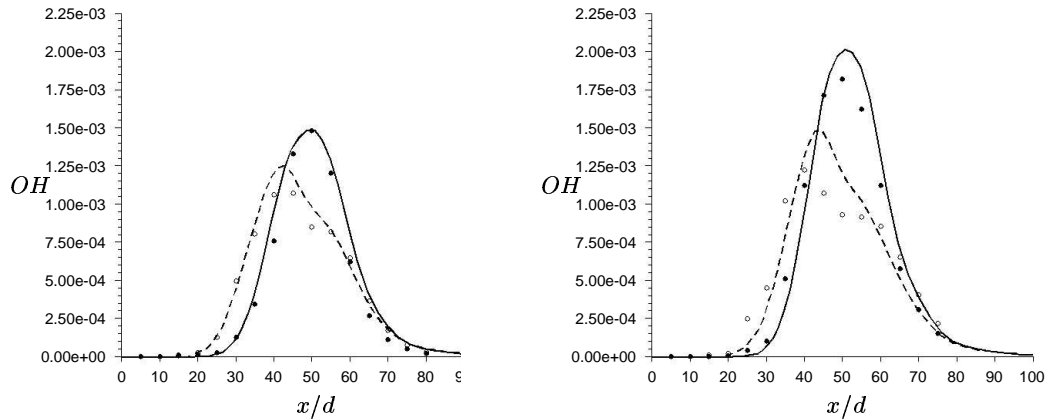


FIGURE 3. Axial plot of mean and RMS OH mass fraction for flame D (left) and flame F (right). Symbols as in Figure 1.

D. Both plots show a slight CO over-prediction in lean mixtures, and substantial CO over-prediction in rich mixtures. The CO over-prediction could be due to contributions from the ignition model, which equilibrates a few points in the LEM field at the start of the simulation, causing initially high CO and H_2 . This artifact is more pronounced at earlier simulation times in the LEM simulation, corresponding to near-nozzle locations in the CFD simulation where the variance is large.

The NO mass fraction in Figure 6 is over-predicted at lean axial down-stream locations. This over-prediction could have contributions from assumptions in the Constructed PDF model, as well as limitations in the original chemical mechanism and its reduction, and limitations in the thin-body radiation model. Figure 7 plots average NO conditional on mixture fraction at axial planes $x/d = 45$ (left) and $x/d = 60$ (right). From the $x/d = 60$ graph it is apparent that the NO over-prediction is confined around the stoichiometric

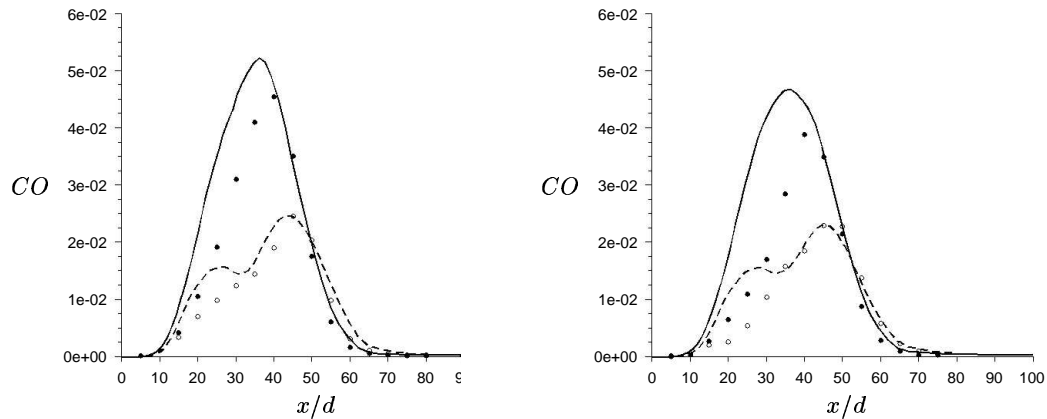


FIGURE 4. Axial plot of mean and RMS CO mass fraction for flame D (left) and flame F (right). Symbols as in Figure 1.

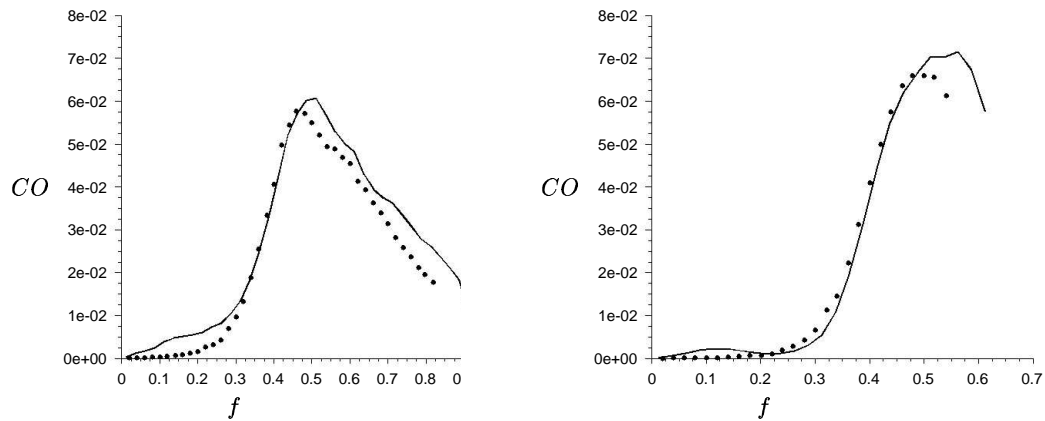


FIGURE 5. Average CO , conditioned on mixture fraction, versus mixture fraction (f) at axial locations $x/d = 30$ (left) and $x/d = 45$ (right), for flame D. Symbols as in Figure 1.

mixture fraction of 0.35. In contrast to the Constructed PDF model, the SLFM predicts NO mass fractions an order of magnitude greater than the measurements, as presented in Figure 8. The error in the SLFM prediction of slow chemical species such as NO is due to disparities in the residence time of the flamelet simulation and the CFD simulation. The flamelet residence time, which is determined by the flamelet strain, will generally not correspond to the residence time in the CFD simulation. In contrast, implicit in the lower moments of the Constructed PDF model (in this case variance of mixture fraction and mean scalar dissipation rate) is a residence time, and a history of entrainment of fuel and oxidizer into reaction zones where NO is accumulated. That is, a given mean mixture fraction, mixture fraction variance and mean scalar dissipation rate correspond to a unique residence time in the non-premixed LEM simulation.

An interesting feature of the Constructed PDF model is the ability to capture local

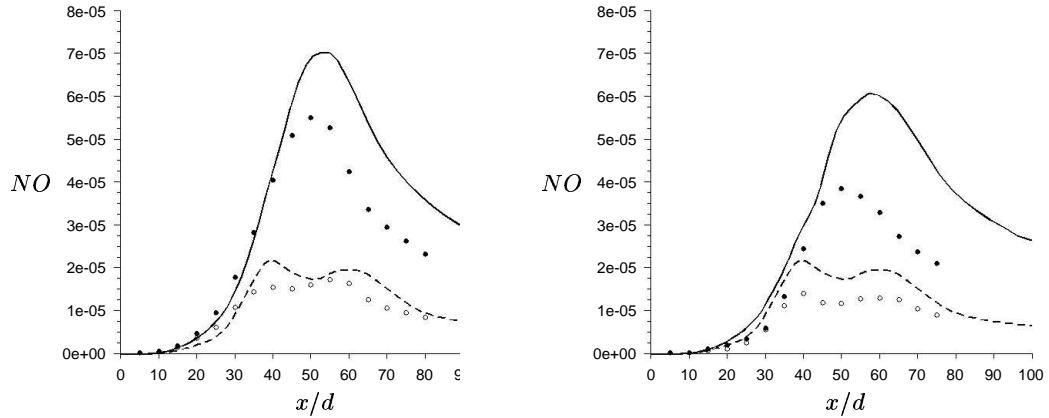


FIGURE 6. Axial plot of mean and RMS NO mass fraction for flame D (left) and flame F (right). Symbols as in Figure 1.

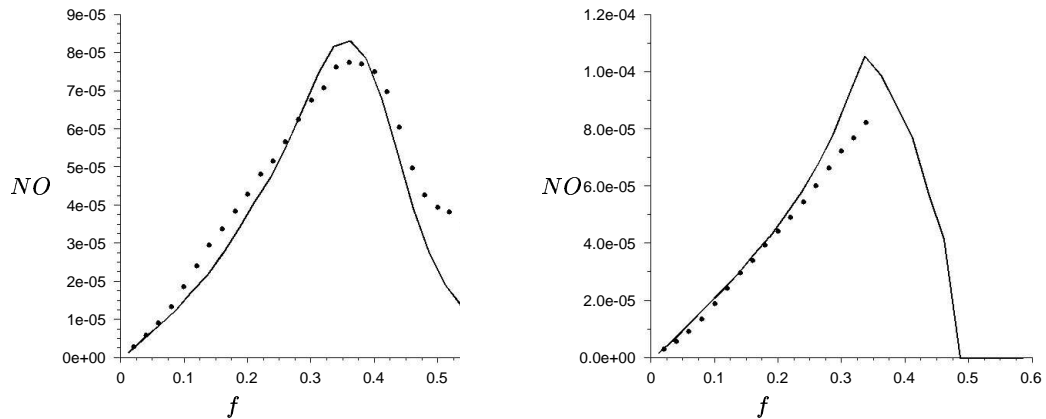


FIGURE 7. Average NO , conditioned on mixture fraction, versus mixture fraction (f) at axial locations $x/d = 45$ (left) and $x/d = 60$ (right), for flame D. Symbols as in Figure 1.

extinction. This is illustrated in Figure 9 which shows scatter plots of temperature in flame F at $x/d = 30$ for the predictions (left) and the experiment (right). The predicted temperatures are obtained from random points in the LEM field, and correspond to the random laser shots of the experiment. Locally extinguished fluid elements are those near the stoichiometric mixture fraction with temperatures well below the equilibrium line. The extent of local extinction is over-predicted in both lean and rich mixtures, which may be due, in part, to the simplified molecular transport assumptions ($Le = 1$). A more accurate modeling of molecular diffusion in the LEM may improve these predictions of local extinction.

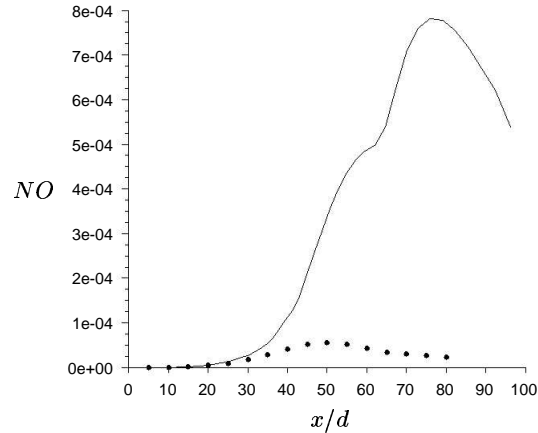


FIGURE 8. Axial plot of mean NO mass fraction for flame D using the Steady Laminar Flamelet Model (SLFM). Symbols as in Figure 1.

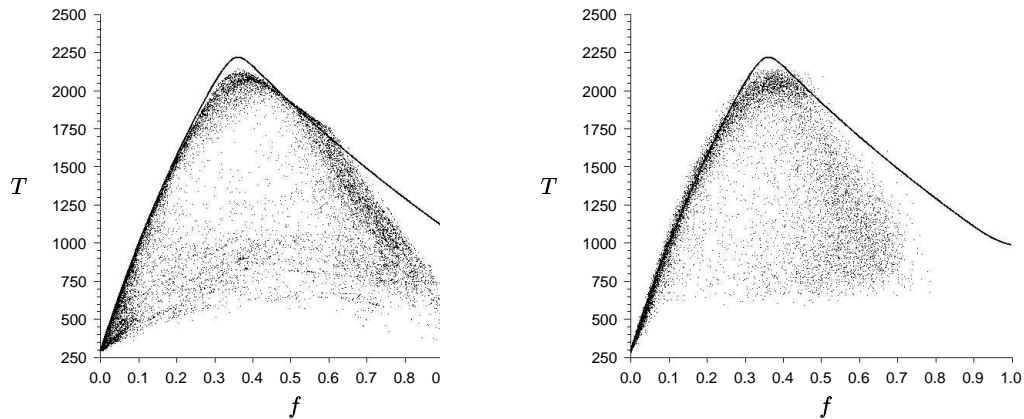


FIGURE 9. Scatter plots of temperature (in degrees Kelvin) versus mixture fraction (f) at $x/d = 30$ for flame F. Predictions (left) and experiment (right) are dots, equilibrium temperature is solid line.

5. Summary and Conclusion

- The Constructed PDF model approximates the joint PDF of species and temperature in an arbitrary geometry reacting flow by the joint PDF of species and temperature calculated in a simple geometry reacting flow.
- Simple geometry simulations are performed over the realizable range of initial conditions, and the thermo-chemical PDF is tabulated as a function of a suitable set of lower moments.
- Once the table is constructed, the PDF is interpolated in a CFD simulation for required lower moments, such as mean and RMS of density, temperature and species mass fractions.

- The Constructed PDF model is similar in this respect to the Steady Laminar Flamelet Model (SLFM) where the turbulence-chemistry interaction is computed *a priori* and tabulated. However, the Constructed PDF model does not assume PDF shapes or chemical state relationships.
- Pre-computing and tabulating the turbulence-chemistry interaction provides very large reductions in the CFD convergence time.
- Scalar decay in homogeneous turbulence is used as the simple geometry, which is modeled with the The Linear Eddy Model (LEM).
- The Constructed PDF model is applied to the prediction of partially-premixed turbulent jet flames, commonly known as Sandia flames D and F.
- A 19 species ARM chemical mechanism (derived from the GRI-Mech 2.11 detailed mechanism) is employed, and ISAT is used to accelerate the chemistry calculations.
- Three lower moments are used to parameterize the PDF, namely mean mixture fraction, mixture fraction variance, and mean scalar dissipation rate.
- Accurate RANS predictions for means and RMS of temperature, major species and *OH* are obtained. *CO* and *NO* predictions agree reasonably well with the measured data, although *CO* is over-predicted in rich regions and *NO* is over-predicted in lean regions.
- Local extinction and re-ignition is captured in the model.

6. Acknowledgements

The first author extends thanks to Dr. Alan Kerstein from Sandia National Labs for several fruitful discussions, and to Drs. Dipankar Choudhury and Nelson Carter from Fluent Inc. for allowing time off to attend the CTR 2004 Summer Program.

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