

A comparative study of Sandia Flame Series (D-F) using sparse-Lagrangian MMC modelling

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Abstract

Sparse-Lagrangian Multiple Mapping Conditioning (MMC) simulations are performed on a turbulent piloted methane jet flame series with increasing levels of local extinction (Sandia Flames D-F). Subfilter conditional scalar dissipation is closed by the generalized MMC mixing model which enforces localisation in the extended space comprising of physical location and a reference mixture fraction which is a filtered field from an LES simulation. A new fractal/gradient model controlling localisation in sparse simulations has been developed recently, and here it is tested on real flame conditions. Using one single localisation constant f_m , simulation results with as few as 1 Lagrangian particle per 27 Eulerian cells show a good match to the measurements; particle number density effects are also explored.

Keywords: Filtered density function, Sparse-Lagrangian simulation, Multiple Mapping Conditioning, Fractal/gradient model

1. introduction

Strong turbulence-chemistry interactions such as found in turbulent combustion with local extinction and re-ignition are the subject of much research, and modelling is made difficult by the non-linearity of reaction rates and the small scales at which the interactions occur. This has implications for large eddy simulation (LES) since the processes which occur at the sub-filter scale and which have to be modelled, are often more important in determining flame structure (especially pollutant formation) than those processes that occur at the resolved scale. Probability density function (PDF) [1] and filtered density function (FDF) methods [2, 3, 4] provide a probabilistic closure of the sub-filter scales while preserving the exact chemical source term. Practical FDF applications usually employ a hybrid method where the FDF is closed at the joint scalar level and is implemented stochastically using Pope particles (Lagrangian particles with properties and a mixing operation [5]),

while exploiting a well resolved turbulent velocity that is simulated by an Eulerian LES. One evident fact of this hybrid method is that the computational cost is linked with the number density of particles. A typical FDF simulation uses 20-50 particles per LES grid cell over a flow domain encompassing a few million LES cells [4]. The cost of simulating engineering scale applications using such conventional intensive-FDF methods is very high.

To make the FDF method accessible to engineering scale problems, the sparse-Lagrangian FDF method, which uses significantly fewer particles than LES grid cells, has been developed in recent years [6] and tested against laboratory flames with moderate to high levels of local extinction [7, 8]. The success of the sparse-Lagrangian method relies on the MMC mixing model which enforces mixing localisation even under the sparse conditions. A particle interaction model is used where particles are selected to form mixing pairs which are close in an extended space of physical location and reference variables. For the diffusion flames cases simulated so far the reference variable is given by the LES filtered mixture fraction as localisation in mixture fraction implies a localisation in the composition space. In non-local mixing models like IEM [9],

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which mixes with a local filtered mean, and Curls model [10], which mixes randomly selected particle pairs from within the same grid cell, the extent of localisation in composition space is determined implicitly by the size of the filter and number of particles that are used; the smaller the filter and the greater the number of particles the better the localisation. Such localisation by numerical intensification is limited by computational resources. If non-local mixing models were applied when using a sparse-Lagrangian FDF model, the distance between mixing particles in composition space would be large. It would result in non-physical mixing of particles across the stoichiometric reaction zone and would likely lead to failure of the model. In contrast, localized mixing models, such as MMC, require that mixing particles in the vicinity of stoichiometry are close in the composition space and thus they give better predictions.

Sparse-Lagrangian MMC has been applied in separate Sandia flame D [7] and E studies [8] at the two most recent past symposia. The modelling relied on a selectable localisation parameter, λ . Problematically λ is not related to the physical quantities of the flow and does not explicitly reveal the localisation structure of the mixing model. Furthermore its value, which was tuned by a priori simulations, varies with the number of particles used. A practical combustion model should have a universal set of parameters, at least for flames within a series such as demonstrated by Xu and Pope [11] and Jones and Prasad [12] for the Sandia series. To this end a new fractal/gradient scale model for localisation of sparse-Lagrangian MMC was introduced [13]. The model parameters are explicitly linked to the localisation structure allowing the distance between mixing particles in the reference mixture fraction space to be directly controlled. This is important, especially for local extinction and re-ignition, because that distance is the most important parameter controlling conditional variance. Simulations of an idealized flame with infinite rate chemistry show that predictions of conditional variance can be obtained by one set of localisation parameters with relative insensitivity to particle number density and flame chemistry [13]. This now needs to be tested for a wide range of real chemistry flame cases. The aims of the present paper are to examine universality of the model parameters for a series of partially premixed methane flames with varying levels of local extinction (Sandia flames D - F) [14]. The major details of the model with emphasis on the

fractal/gradient localisation model are presented in the next section, followed by a description of the simulation case in section 3. Results addressing the aims of the paper appear in section 4. Finally conclusions are drawn in section 5.

2. The model

The computational model adopted in this comparative study is the same as the one previously developed for the separate Sandia flame D [7] and E studies [8] and presented in detail in [13]. A brief overview of the hybrid LES / sparse-Lagrangian MMC model is given here and readers are directed to the previous publications for complete details. The model involves an Eulerian LES with a dynamic Smagorinsky turbulent viscosity model for the filtered velocity and reference mixture fraction fields and a stochastic Lagrangian model for the reactive scalars. Density feedback from the Lagrangian to the Eulerian scheme uses an adapted conditionally averaged form of the equivalent enthalpy method originally developed by Muradoglu et al. [15] and used in intensive-Lagrangian FDF simulations by Raman and Pitsch [4]. The adapted density feed back method matches the conditional means of the Eulerian and Lagrangian submodels. It is fully documented and tested against flames with real and ideal chemistry in Refs.[8, 13].

In the FDF model the subfilter conditional scalar dissipation is closed through a particle mixing model. Particle mixing pairs are selected by an approximate minimization of the normalized square distance in extended physical and reference mixture fraction, $(x, \tilde{f})$, space [8]:

$$\hat{d}_{(p,q)} = \left[\sum_{j=1}^3 \left(\frac{d_{(x_j)}^{p,q}}{r_m} \right)^2 + \left(\frac{d_{(f^*)}^{p,q}}{f_m} \right)^2 \right]. \quad (1)$$

In (1) asterisks denote stochastic quantities assigned to or evaluated at the particles and $d_{(\cdot)}^{p,q} = |(\cdot)^p - (\cdot)^q|$. The parameters r_m and f_m are characteristic scales in the physical and reference spaces, respectively. In the previous publications [8] they were set as the geometric scales of the flow; r_m was set as the nozzle radius and $f_m = 1/\lambda$, where λ was the localisation control parameter. As discussed above a new fractal/gradient model [13] is to be used here. The model links the scales r_m and f_m by considering isoscalar contours in a turbulent field as fractal surfaces. A mixing particle pair is selected

so that both particles lie close to the same fractal surface such that they are separated by a small distance, f_m , in reference mixture fraction space. By equating the volume subtended by the particle pair and the volume of fluid represented by each particle (as defined by the particle number density) it is found that

$$r_m = c_m \left(\frac{d\tilde{f}}{dn} \frac{\Delta_L^3}{\Delta_E^{2-D}} \frac{1}{f_m} \right)^{1/D}. \quad (2)$$

Here c_m is a constant, $d\tilde{f}/dn$ is the gradient of the reference mixture fraction normal to the fractal surface, Δ_L is the nominal distance between particles (linked to the particle number density), Δ_E is the LES filter width and D is the fractal dimension. Fractal properties in turbulence are discussed in a number of publications [16, 17]. The computational fractal dimension that achieves good control of mixing distances over a range of sparse conditions [13] seems to match the experimentally observed fractal dimension of 2.36 [16]. Comparison between predicted (from Eq.(2)) and numerically observed inter-particle distances from our previous simulations indicated that $c_m = 0.5$. Note that c_m is not related to the micromixing timescale as, say, C_ϕ is in RANS-PDF models. In sparse simulations in LES the mixing timescale is determined by the scaling laws of the inertial interval. That modelling is documented in detail elsewhere [8].

We now see that the scales r_m and f_m can be linked to each other through Eq.(2) rather than arbitrarily to the geometric scales of the flow and λ as was previously the case [8]. f_m represents a characteristic distance in mixture fraction space between mixing particles and is selected by the user; a very small value would suppress conditional fluctuations and produce a model with similar properties to first-order conditional moment closure [18] whereas larger values of f_m yield larger conditional variances. The optimal value of f_m will depend on the flame regime (i.e. how well the fluctuations of the mixture fraction define the turbulence-chemistry interactions). An analysis of the distances between mixing particles of our past simulations [8] indicates that $f_m = 0.03$ should be used for the partially premixed methane flames in the Sandia series. Since in the new fractal/gradient model r_m is a characteristic physical distance between mixing particles it is the characteristic Lagrangian filter width.

As previously described [7] the mixing particle selection algorithm approximately minimizes $\hat{d}_{(p,q)}$

using a kd-tree method which requires global parameters for f_m and r_m . Therefore we calculate a global value of r_m based on the quantities in Eq.(2) at a characteristic point in the flow. We use the nozzle exit since this is a well defined point where the scalar gradient $d\tilde{f}/dn$ is defined by the boundary conditions and is the same for all three flames in the Sandia series.

3. Simulation details

The comparative study using sparse-Lagrangian MMC is performed for the well documented Sandia Flame series D-F [14]. This series has increasing jet velocities and exhibits increasing levels of local extinction with flame F being close to blow-off. The burner has a central fuel nozzle of diameter $d = 7.2$ mm surrounded by a pilot that extends to a diameter of 18.2 mm. The jet fuel is 25% CH₄ and 75% air by volume and has a stoichiometric mixture fraction of $Z_{st} = 0.351$. The pilot burns a lean premixture with the same nominal enthalpy and equilibrium composition as methane/air at an equivalence ratio of 0.77. The bulk jet velocities are 49.9, 74.4 and 99.2 m/s for flames D, E and F, respectively. The corresponding pilot inlet velocities are 11.4, 17.1 and 22.8 m/s.

The hybrid Eulerian LES/sparse-Lagrangian MMC model is implemented numerically within the Flowsi LES code [19] as documented in earlier publications [6, 7]. The cylindrical simulation domain extends axially to $L_{axial} = 0.25$ m (35 jet diameters) and radially $L_{rad} = 0.25$ m. The mesh used consists of $512 \times 55 \times 32$ in the axial, radial and azimuthal directions, respectively. The smallest finite volume cells in the simulation at the flame axis are $0.5\text{mm} \times 0.5\text{mm} \times \pi/32\text{rad}$. In the sparse-Lagrangian MMC we use 1 particle per 27 Eulerian LES cells (1L/27E). The characteristic distance between particles at the jet axis is approximately 1.6 mm. After a steady-state has been reached, stationary statistics are accumulated over eight characteristic domain flow through times. Chemical source terms are obtained from a detailed kinetics scheme (GRI-3.0) [20] containing 34 species and 219 reactions (NO_x excluded). To test sensitivity of the model to the Lagrangian filter width (characterized by r_m), one additional simulation is run for flame F using 1 particle per 8 LES cells (1L/8E). We chose this case because it is the most difficult of the three flames and predictions are most sensitive to variations in the model.

4. Results

To best demonstrate the extinction and re-ignition phenomena, results are taken from $x/d = 7.5$ and 15 where strong extinction is evident and $x/d = 30$ where re-ignition has occurred. Unless otherwise noted predictions are from the 1L/27E simulations. Some figures also contain 1L/8E predictions and these will be discussed towards the end of the results section.

The MMC model allows for quite direct control of the conditional variance. This is done by controlling the distance between mixing particles in the reference mixture fraction space. Fig.1 shows the numerically observed mean distance between mixing particles in that space, $\langle d_{f^*} \rangle$, for all three flames. Note that the relationship between $\langle d_{x^*} \rangle$ and $\langle d_{f^*} \rangle$ is the same as between r_m and f_m given in Eq.(2) just that the former are the actual mean values of mixing distances in physical and reference mixture fraction spaces at different locations while the latter are the characteristic values used to select mixing particle pairs in Eq.(1). It can be seen from the figure that $\langle d_{f^*} \rangle$ peaks around the shear layer where the scalar gradient, $d\tilde{f}/dn$, is largest. For 1L/27E simulations $\langle d_{f^*} \rangle$ for all three flames are in good agreement with each other. Close to the nozzle exit location, $x/d = 0.5$, the maximum value of $\langle d_{f^*} \rangle$ is reasonably well controlled to 0.03 which is the preset characteristic value for the model parameter, f_m . It needs to be pointed out that $\langle d_{f^*} \rangle$ varies by a lot at different locations in the flow according to the magnitude of the scalar gradient. The dip at $r/d = 1$ at the nozzle exit coincides with the pilot where the scalar gradient is near zero.

Figure 2 shows radial profiles of the mean and rms of the mixture fraction for all three flames. Note this is the actual mixture fraction determined from the sparse-Lagrangian MMC 1L/27E simulation and not the reference mixture fraction given by the Eulerian LES. An excellent agreement between the simulations and experiments are achieved in both flames D and E at all axial locations. Flame F is the most difficult of the cases to model correctly due to its being close to blow-off (discussed in more detail below). The mixture fraction predictions for the flame F case appear to be less diffusive than the experiment which might be attributed to a slight under prediction of extinction for flame F (see discussion below) which in turn implies higher temperatures and lower density than the experiments yielding slightly slower decay of the jet core.

The predicted and experimental scatter plots of temperature versus mixture fraction at different locations for all three cases are shown in Fig. 3-5 and their conditional mean values are shown later in Fig. 6. With increasing jet velocity, the flame series exhibit an increasing level of extinction, most evident in Flame E and F at $x/d = 7.5$ and 15 . Predictions for flames D and E are in very good agreement with the experimental data. There are slightly fewer conditional fluctuations evident in the predicted scatter plots for flame D than in the experiments but this flame has very low conditional variance anyway and conditional means are in excellent agreement at all three axial locations. As a close to blow-off flame, the bimodal nature of Flame F is clearly captured in the predicted scatter plot at $x/d = 15$; there is an upper flamelet band and a lower close to extinction band which peaks at about 1000K. For the Flame F simulation, the scatter plot at $x/d = 30$ predicts an earlier re-ignition relative to the experiments. Similar discrepancy has also been reported by others [12]. In our simulations great care was required to avoid the occurrence of isolated turbulent events where the temperature of a small number of particles departed a great distance from the mean that then lead to global extinction; this is particularly important for very sparse simulations where each particle represents a significant mass of fluid. We tried increasing f_m above 0.03 to better capture the level of local extinction in flame F. While this led to more pleasing scatter plots for flame D it caused flame F to globally extinguish due to such rare turbulent events that in some cases would occur a few domain flow through times into the simulation after the steady state had (apparently) already been reached. Another issue is that we use f_m as a global value. The scatter plots for flame F reveal reasonable agreement with experiments at $x/d = 7.5$ and 15 but the less satisfactory result at $x/d = 30$ suggests a larger value of f_m may be required there. Having f_m determined by local parameters rather than global characteristic parameters is possible in principle but has not been tested here.

The conditional means of the reactive scalars CO_2 and CO are shown in Fig. 9 and 10 for the 1L/27E simulations. Again a very good agreement between simulation and experiment results are achieved for flames D and E; there is slight over-prediction of rich side CO in flame E. In the flame F results only the fuel lean side is well matched, however, in line with the temperature results dis-

cussed above the stoichiometric and rich side values are over-predicted. The unconditional mean and rms profiles of CO_2 and CO are shown in Fig. 7 and 8. In general there is very good agreement between the predicted and measured results, although there is an over-prediction of the intermediate CO in flame F corresponding to the conditional average results.

The above comparative results are from simulations with 1 particle per 27 Eulerian cells (1L/27E). Most importantly the results demonstrate that a single value of f_m produces generally good results for all flames in the Sandia series. An advantage of sparse methods is the ability to control the number of particles and to balance computational cost and level of detail in the predictions (e.g. stationary statistics can be achieved with very few particles while larger numbers of particles are needed to accurately observe local and instantaneous filtered means [13]). The new fractal/gradient localisation model attempts to allow the same value of f_m to be used for simulations with different numbers of particles. The aim is to keep f_m the same regardless of the number of particles used while r_m varies in a known way according to Eq.(2). Here this is tested by an additional 1L/8E simulation for flame F. Since particle number density is increased r_m becomes smaller. This can be viewed as a reduction in the characteristic Lagrangian filter width. Since r_m is changed, the 1L/8E simulation is not a numerical convergence test but rather a model sensitivity test. Note that numerical convergence in sparse methods while keeping the Lagrangian filter width constant is discussed theoretically in Ref.[5]. Fig.1 (discussed previously) shows that $\langle d_{f^*} \rangle$ for 1L/8E is very similar to that for the 1L/27E simulation though for 1L/8E there are slightly smaller peak values. This very minor discrepancy is probably caused by numerical noise in the particle number control algorithm [7]; in very sparse simulations the relative fluctuations of particle number density are larger. The conditional and unconditional means predicted by the 1L/8E simulation are shown alongside the 1L/27E predictions in Fig.6 through 8. We see that overall there is a reasonable similarity between the results although there are some local differences. At $x/d = 7.5$ and 30 the agreement is excellent but there is discrepancy at $x/d = 15$ which is the point in the flame with maximum local extinction. These results seem to indicate that up to a certain level of local extinction (i.e. the extent seen at $x/d = 7.5$) the distance in mixture frac-

tion space between mixing particles is the most important model parameter for controlling conditional variance and predictions are relatively insensitive to the physical distance between mixing particles (characterized by r_m). Beyond that level of local extinction (i.e. the extent seen at $x/d = 15$) it is not enough just to control the mixing distance in mixture fraction space by the single global parameter f_m ; other quantities play a more significant role e.g. physical distance, progress variable. This is perhaps not too surprising since heavy local extinction means that there is less of a correlation between fluctuations of mixture fraction and reactive species.

5. Conclusion

The Sandia Flame Series D-F have been simulated using the sparse-Lagrangian MMC method. The detail of the localisation structure in the MMC mixing model are controlled according to the physically-based fractal/gradient scaling model to maintain the same distance in reference mixture fraction space between mixing particles in all three cases. This model also allows adjustment for particle number density. When f_m is set to 0.03 conditional and unconditional reactive scalar results for flames D and E are in very good agreement with experimental data at all locations. For flame F, which is close to blow-off, results are qualitatively correct, the bimodal nature of the extinction is captured, but there is an early prediction of re-ignition. Importantly the increased level of extinction arising from the increasing jet velocity are successfully captured by the model with a single value of f_m . The sensitivity of the model to the physical distance between mixing particles has been analyzed with a more intensive 1L/8E simulation for the most difficult case (flame F). Although the fractal/gradient model effectively controls the distance in reference mixture fraction space between mixing particles the reactive scalar predictions at the location with strongest local extinction differ. The sensitivity is not observed at other locations with less local extinction. Clearly where there is heavy extinction localness of mixing in mixture fraction space does not ensure localness in composition space as well as it does for flames D and E with less extinction. This problem may be overcome by the incorporation of an additional reference variable such as sensible enthalpy as has been one in the past for the deterministic form of MMC.

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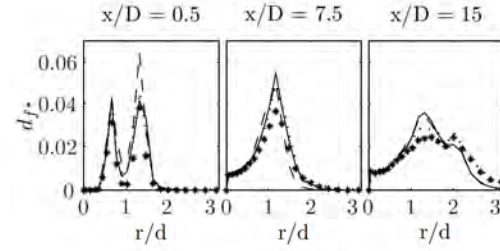


Figure 1: Radial profiles of steady-state mean distance in mixture fraction space between mixing particles. Solid line, flame D; dashed line, flame E; dotted line, flame F; star, flame F with 1L/8E.

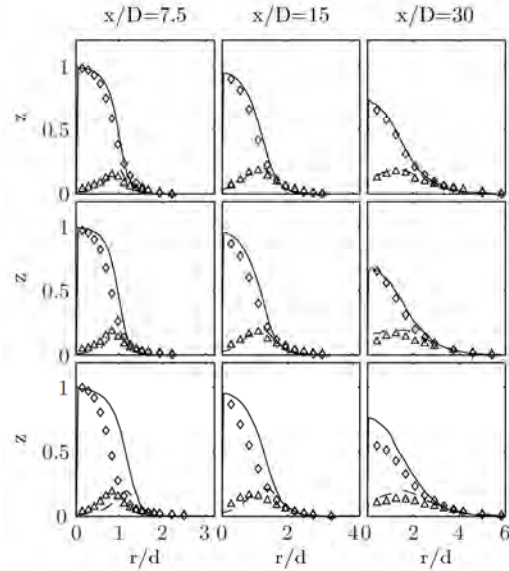


Figure 2: Radial profiles of steady-state mean and rms for mixture fraction. Open symbols, experimental data; lines, 1L/27E simulation results. From top to bottom are flame D, flame E and flame F results

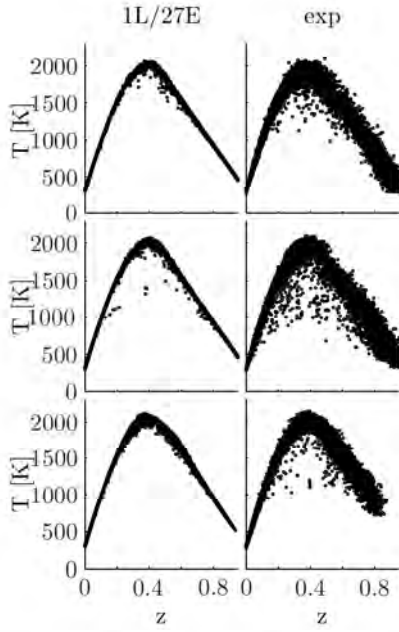


Figure 3: Scatter plots of temperature versus mixture fraction for flame D. Top, $x/d = 7.5$; middle, $x/d = 15$; bottom, $x/d = 30$.

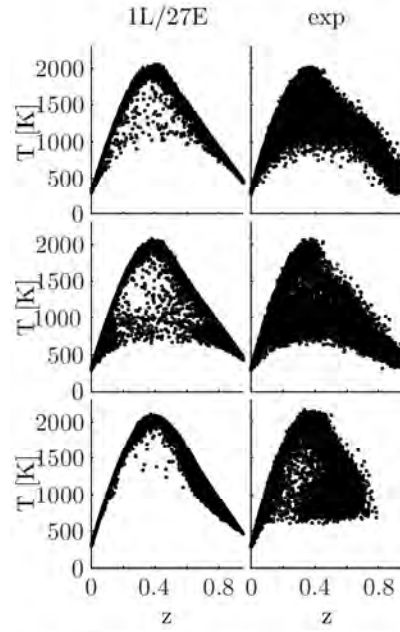


Figure 5: Scatter plots of temperature versus mixture fraction for flame F. Top, $x/d = 7.5$; middle, $x/d = 15$; bottom, $x/d = 30$.

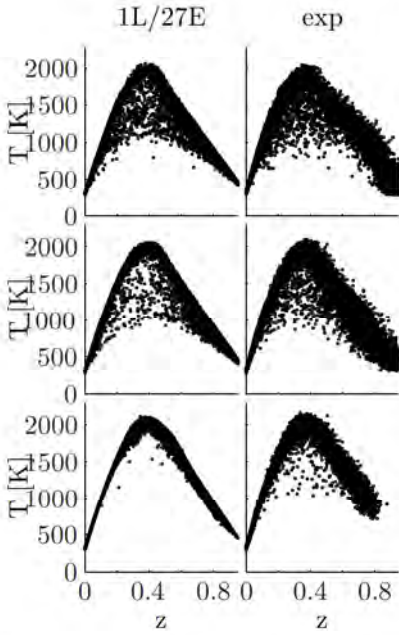


Figure 4: Scatter plots of temperature versus mixture fraction for flame E. Top, $x/d = 7.5$; middle, $x/d = 15$; bottom, $x/d = 30$.

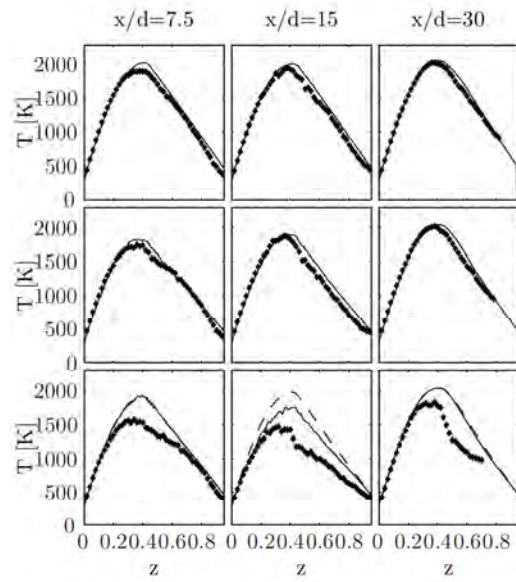


Figure 6: Conditional mean temperature versus mixture fraction. From top to bottom are flame D, flame E and flame F results. Open symbols, experimental data; solid lines, simulation results; dashed-lines, results for flame F with 1L/8E

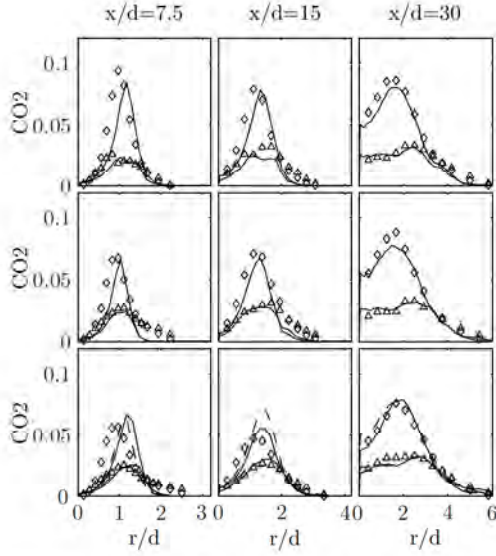


Figure 7: Radial profiles of steady-state mean and rms for CO_2 . From top to bottom are flame D, flame E and flame F results. Open symbols, experimental data; solid lines, simulation results; dashed-lines, results for flame F with $1L/8E$.

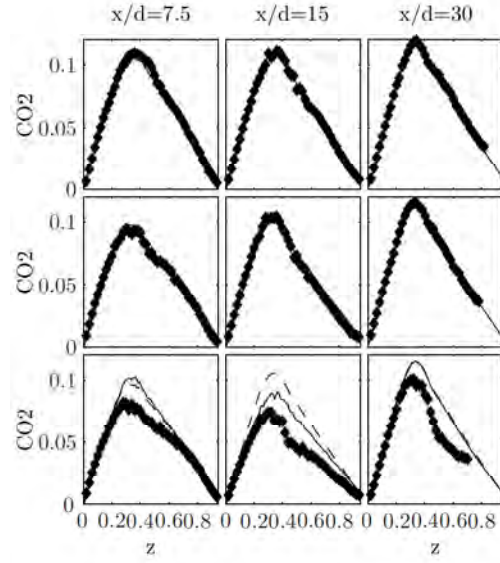


Figure 9: Conditional mean CO_2 versus mixture fraction. From top to bottom are flame D, flame E and flame F results. Open symbols, experimental data; solid lines, simulation results; dashed-lines, results for flame F with $1L/8E$.

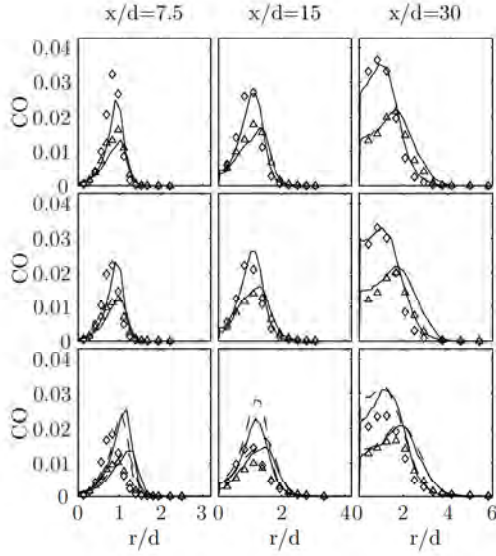


Figure 8: Radial profiles of steady-state mean and rms for CO . From top to bottom are flame D, flame E and flame F results. Open symbols, experimental data; solid lines, simulation results; dashed-lines, results for flame F with $1L/8E$.

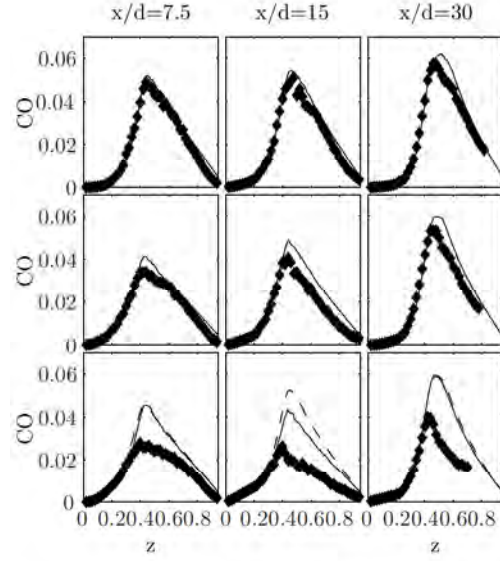


Figure 10: Conditional mean CO versus mixture fraction. From top to bottom are flame D, flame E and flame F results. Open symbols, experimental data; solid lines, simulation results; dashed-lines, results for flame F with $1L/8E$.