Piloted CH$_4$/Air Flames C, D, E, and F – Release 2.1

15-JUN-2007

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INTRODUCTION

This file (SandiaPilotDoc21.pdf) provides documentation for the 1997 Sandia data set of multiscalar measurements in piloted methane-air jet flames [1] stabilized on a burner developed by Sydney University [2]. This information is made available as part of the *International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames* [3] to facilitate collaborative comparisons of measured and modeled results for selected turbulent flames. The "preliminary" data release, which came before the TNF3 Workshop in 1998, included results for flame D only. Scalar data from four piloted flames (C, D, E, and F) have been available by request since January 1999. These flames have increasing velocity in the main jet and pilot and increasing probability of localized extinction. The archive of scalar data (pmCDEF.zip or pmCDEF.tar.Z) included with this release is the same as that provided previously by request. The purpose of Release 2.0 (January, 2003) was to expand the documentation to cover these four flames and update some aspects of the velocity boundary conditions. The only change in this file, with Release 2.1, is the addition of Reference [14], which presents previously unpublished results from the original experiments and describes long (6000-shot) records from flame D.

Measured scalars include temperature, mixture fraction, N$_2$, O$_2$, H$_2$O, H$_2$, CH$_4$, CO, CO$_2$, OH, and NO. CO is measured by Raman scattering and by LIF. The CO-LIF measurements are more accurate and should be used in comparisons with models. The data set includes axial and radial profiles of Reynolds- and Favre-average mass fractions and rms fluctuations, conditional statistics at each streamwise location, and complete single-shot data for all measured scalars. Data included here and used for all TNF Workshop comparisons were obtained during the same experimental series as those reported by Barlow and Frank [1], but on different days, allowing for detailed mapping of each flame. Experimental methods and measurement uncertainties are outlined in [1] and further described in [4]. Data from flames A (laminar) and B (transitional) are not included in this archive. Two component laser-Doppler anemometry (LDA) measurements in flames D, E, and F were performed at the Technical University of Darmstadt by Christoph Schneider et al. [5], and those data are available separately as noted below.

Flames D, E, and F have been modeled by several groups, and a partial list of modeling papers on these flames is provided in the reference list [6-10]. The Proceedings of the TNF3, TNF4, and TNF5 Workshops [3] include numerous graphical comparisons of measured and modeled results, as well as summaries of the modeling approaches used.

USE OF THE DATA

Please contact R. Barlow if you use or publish these data and are not already on the TNF email distribution list. This will ensure that you will receive notification regarding TNF Workshop data sets and activities.

Averaged results and scatter plots of temperature and species mass fractions from these piloted flame experiments have already been widely published in modeling papers. No special permission is needed to include these data in further publications. However, we are preparing a paper (long overdue) on aspects of the data that have not yet been published, including such things as transport effects (turbulent stirring vs. differential molecular diffusion), radial variations in conditional statistics, and deviations from partial equilibrium [4]. Therefore, we request that researchers contact us *before* presenting or publishing any further statistical analysis of the scatter data for these flames.

NOTICE

This data release was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of the contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof or any of their contractors or subcontractors.

GENERAL DESCRIPTION OF THE FLAMES

The burner geometry is the same as used in numerous previous investigations of piloted flames at Sydney University and Sandia [1,2]. The jet fluid is a mixture of three parts air and one part CH_4 by volume. This mixture significantly reduces the problem of fluorescence interference from soot precursors, allowing improved accuracy in the scalar measurements. Partial premixing with air also reduces the flame length and produces a more robust flame than pure CH_4 or nitrogen-diluted CH_4. Consequently, the flames may be operated at reasonably high Reynolds number with little or no local extinction, even with a modest pilot. The mixing rates are high enough that these flames burn as diffusion flames, with a single reaction zone near the stoichiometric mixture fraction and no indication of significant premixed reaction in the fuel-rich CH_4/air mixtures.

Flame D (Re=22400) has a small degree of local extinction [1]. It was selected as the initial target for TNF3 comparisons because high Reynolds number is desirable for model validation

and the small probability of local extinction allows for useful comparisons with models that do not include extinction. Flames E and F have significant and increasing probability of local extinction above the pilot region, with flame F being close to global extinction of the downstream part of the flame.

The pilot is a lean (phi=0.77) mixture of C_2H_2, H_2, air, CO_2, and N_2 with the same nominal enthalpy and equilibrium composition as methane/air at this equivalence ratio. The flow rates to the main jet and the pilot are scaled in proportion for the C-F series, so that the energy release of the pilot is approximately 6% of the main jet for each flame. The burner exit was positioned approximately 15 cm above the exit of the vertical wind tunnel in the TDF laboratory. The flames were unconfined.
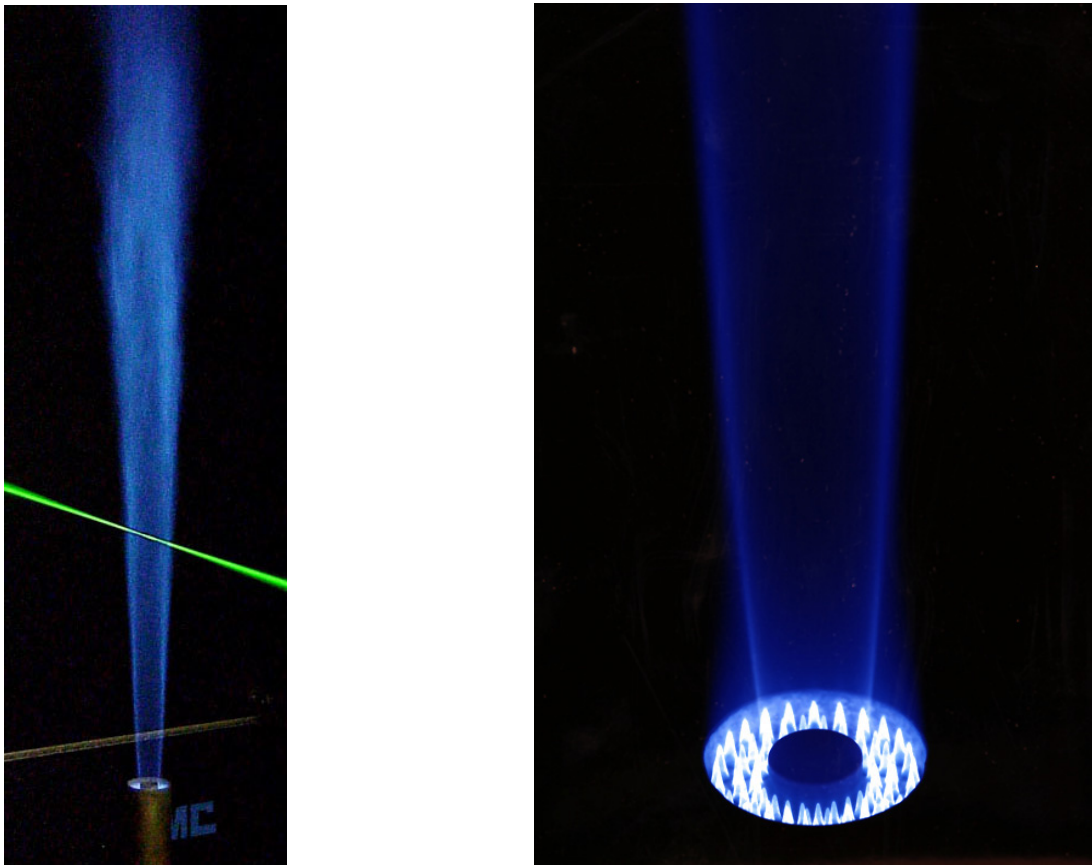

Fig. 1. Flame D (left) with Nd:YAG laser beam and close-up of the pilot flame (right).

BURNER DIMENSIONS

```
Main jet inner diameter, d   = 7.2 mm
Pilot annulus inner diameter = 7.7 mm  (wall thickness = 0.25 mm)
Pilot annulus outer diameter = 18.2 mm
Burner outer wall diameter   = 18.9 mm (wall thickness = 0.35 mm)
Wind tunnel exit             = 30 cm by 30 cm
```

BULK FLOW AND SCALAR BOUNDARY CONDITIONS

```
Coflow velocity  (Ucfl)       = 0.9 m/s (+/- 0.05 m/s) @ 291 K, 0.993 atm
Main jet composition          = 25% CH4, 75% dry air by volume
Main jet kinematic viscosity  = 1.58e-05 m^2/s (from chemkin)


Main jet velocity @ 294K, 0.993 atm:
                    Ubulk_C  = 29.7 m/s (+/- 2 m/s)
                    Ubulk_D  = 49.6 m/s (+/- 2 m/s)
                    Ubulk_E  = 74.4 m/s (+/- 2 m/s)
                    Ubulk_F  = 99.2 m/s (+/- 2 m/s)
```

Elemental mass fractions in the jet and coflow that are used in calculating the mixture fraction are given below, under the definition of mixture fraction.

The flame stabilizer in the pilot is recessed below the burner exit, such that burnt gas is at the exit plane, as shown in Fig. 1. The compositional boundary condition in the pilot for flame D was determined by matching the measurements at x/d=1 with calculations (by J-Y Chen) of laminar unstrained premixed CH_4/air flames and then extrapolating to the conditions at burner exit plane, based on the estimated convective time up to x/d=1. The pilot burnt gas velocity is determined from the cold mass flow rate, the density at the estimated exit condition, and the flow area of the pilot annulus. The resulting pilot flame boundary conditions are tabulated below. Separate calculations were performed to demonstrate that there are negligible differences in burnt gas composition for the pilot mixture vs. CH_4/air at the same total enthalpy and equivalence ratio.

The pilot composition measured in the (nearly) flat portion of the radial profile at x/d=1 in flame D is:

```
phi        = 0.77
Fch        = 0.27
Yn2        = 0.734
Yo2        = 0.056
Yh2o       = 0.092
Yco2       = 0.110
Yoh        = 0.0022
```

The pilot composition at the burner exit for flame D is taken as that of an unstrained CH_4/air premixed phi=0.77 flame at the point in the flame profile where T=1880 K, following the process outlined above.

```
phi        = 0.77              Yh2        = 1.29e-4
Fch        = 0.27              Yh         = 2.48e-5
T          = 1880 K (+/- 50 K) Yh2o       = 0.0942
rho        = 0.180 kg/m^3      Yco        = 4.07e-3
Yn2        = 0.7342            Yco2       = 0.1098
Yo2        = 0.0540            Yoh        = 0.0028
Yo         = 7.47e-4           Yno        = 4.8e-06
```

We note that a similar composition (within experimental uncertainty) is obtained from a laminar diffusion flame calculation with the present fuel-air boundary conditions, equal species diffusivities, and a relatively low strain rate (a ~ 20/s) at 0.27 mixture fraction. We also note that this analysis to estimate the pilot composition at the exit plane has not been performed for the other flames.

Figure 2 shows that the measured pilot temperature in the flat region of the profile at x/d=1 is lower in flame F than in flames D and E. Temperature measurements at the near-nozzle locations (x/d=1,2,3) are somewhat less accurate than those further downstream because they are determined from Raman results (total number density) rather than Rayleigh scattering, and the differences are within the uncertainty in the temperature measurement. The same can be said for the small differences in measured pilot composition for these flames. As far as we are aware, the scalar composition given here for the flame D pilot has been used for most model calculations of flames E and F. This seems appropriate. However, the sensitivity of model predictions to uncertainty the pilot boundary conditions is an important consideration, as noted by Tang et al. [7], especially with regard to results for flame F, which is very close to global extinction.

The pilot bulk velocities corresponding to the above-specified conditions, the flow area of the pilot annulus, and the measured mass flow rates for the four flames are:

```
Uplt_C = 6.8 m/s (+/- 0.3 m/s)
Uplt_D = 11.4 m/s (+/- 0.5 m/s)
Uplt_E = 17.1 m/s (+/- 0.75 m/s)
Uplt_F = 22.8 m/s (+/- 1.0 m/s)
```
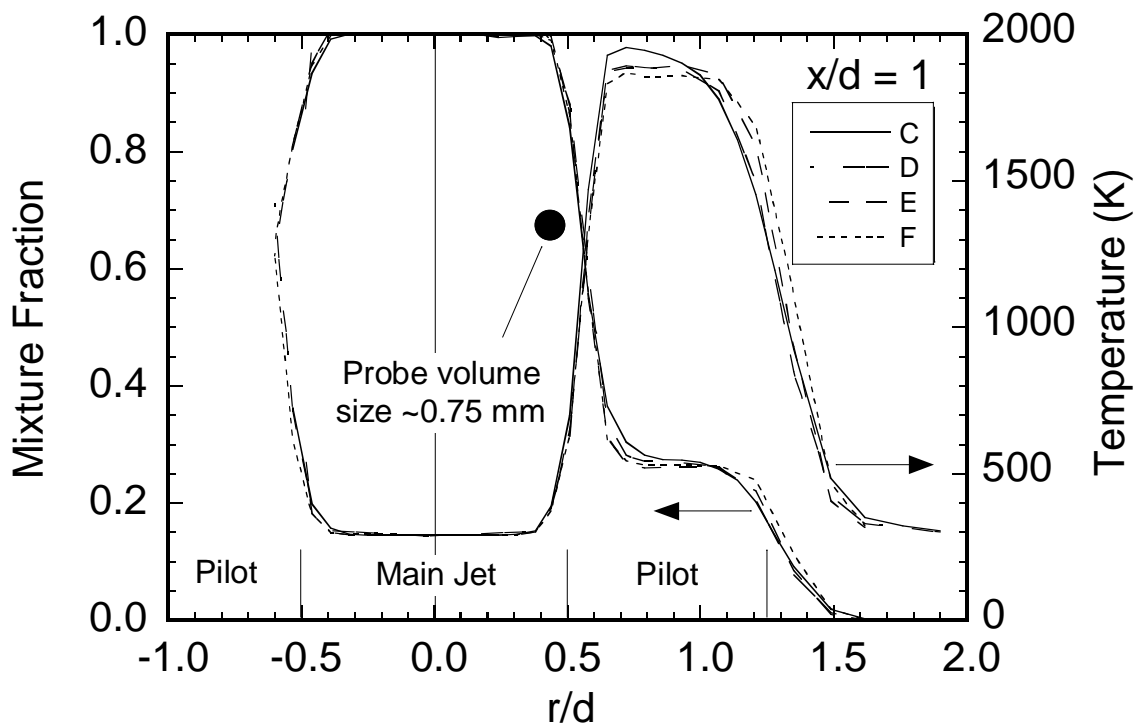

Fig. 2. Measured radial profiles of Favre-average mixture fraction and temperature at x/d=1 in the four turbulent piloted flames.

VELOCITY BOUNDARY CONDITIONS

Two component velocity measurements were performed at the Technical University of Darmstadt by Christoph Schneider et al. [5]. Complete velocity data are available from TU Darmstadt.

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                    http://www.tu-darmstadt.de/fb/mb/ekt/flamebase.html

Measured axial velocity and turbulence intensity are tabulated below, and we emphasize here that this is an update of the profile given in the documentation file for the "preliminary" release of the flame D data, which was posted on the TNF site until February 2003.

R/D[-]	<U>[m/s]	<u`u`>[m2/s2]	
0.0000	62.95	6.13	OBTAIN COMPLETE 2-COMPONENT
0.0694	62.54	6.23	DATA FROM TU DARMSTADT
0.1388	61.36	8.27	
0.2083	59.21	12.45	
0.2777	56.73	15.93	
0.3472	53.34	20.66	
0.4166	48.80	24.50	
0.4861	41.99	37.40	
0.5000	0.00	0.00	
0.5555	3.45	0.322	
0.6250	11.46	1.736	
0.6944	15.18	1.484	
0.7638	15.45	1.586	
0.8333	15.15	1.797	
0.9027	15.97	1.360	
0.9722	15.56	1.476	
1.0416	15.42	1.410	
1.1111	15.04	1.546	
1.1805	14.25	1.875	
1.2300	10.96	1.508	
1.2400	0.00	0.000	
1.3194	1.04	0.009	
1.3888	1.01	0.007	
1.4583	1.07	0.007	
2.1041	1.02	0.006	

The velocity profiles from the preliminary release have been used in some model calculations, while others have used the measured profile from TUD. Merci et al. [12] report little difference between results using these different inlet profiles. However, we include the old profiles below to allow other to make similar comparisons. The pilot velocity profile was originally assumed to be flat, except for thin boundary layers. A piecewise-linear profile was specified that takes the half velocity points to be mid-way across the burner walls, such that the thickness of the inner and outer walls is neglected. The boundary layer in the coflow is taken to have the same shape as specified by Sydney University, except that the profile was shifted to correspond to the measured 18.9-mm outer dimension of the burner. Also, a free stream turbulence intensity of 1% was assumed. Reference velocities for the old profiles are: Uc,o=63.1 m/s, Uplt=11.4 m/s, and Ucfl=0.9 m/s. Old and new profiles of mean velocity are compared in Fig. 3.
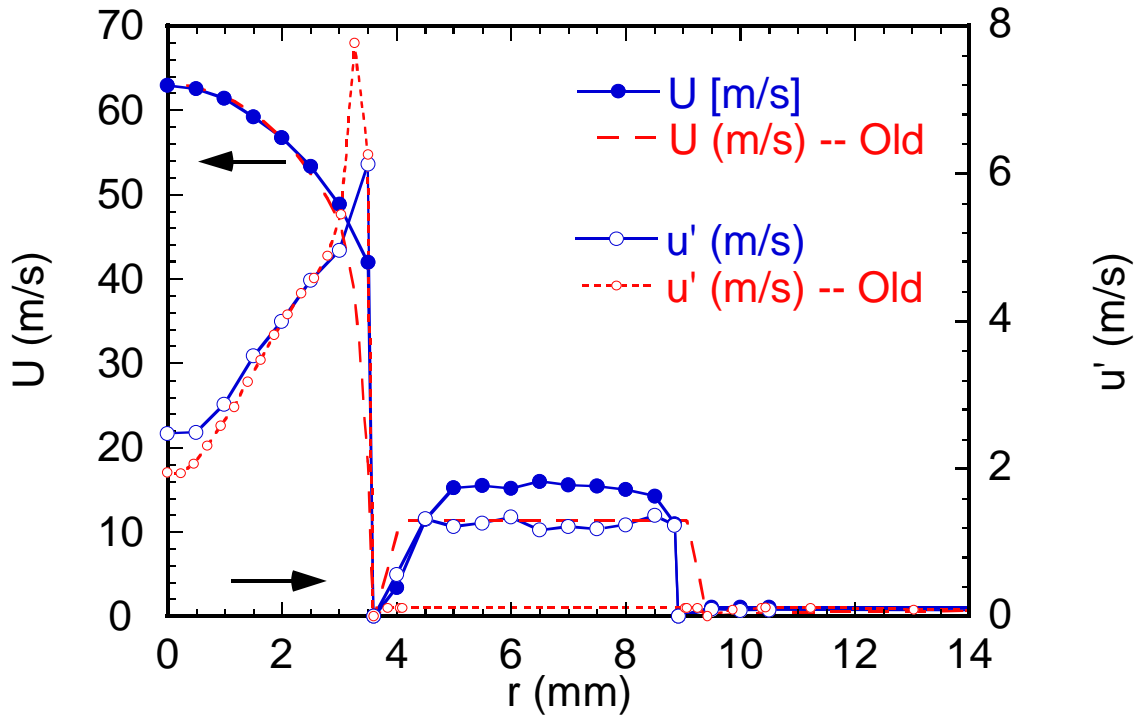
Fig. 3. Comparison of current and old velocity profiles.

```
r/R      U/Uc,o  u'/Uc,o    OLD JET PROFILE FROM PRELIMINARY RELEASE
0.000    1.000   0.0309
0.065    0.999   0.0307
0.130    0.995   0.0327
0.194    0.988   0.0366
0.259    0.978   0.0409
0.324    0.967   0.0450
0.389    0.951   0.0504
0.453    0.933   0.0550
0.518    0.912   0.0604
0.583    0.887   0.0648
0.648    0.858   0.0693
0.712    0.824   0.0726
0.777    0.785   0.0773
0.842    0.732   0.0863
0.907    0.613   0.1230
0.972    0.291   0.0991
1.000    0.000   0.0000


r/R      U/Uplt  u'/Uplt    OLD PILOT PROFILE FROM PRELIMINARY RELEASE
1.00     0.00    0.00
1.07     0.50    0.01
1.13     0.99    0.01
1.14     1.00    0.01
2.51     1.00    0.01
2.52     0.99    0.01
2.57     0.50    0.01
2.62     0.00    0.00
```

```
     r/R     U/Ucfl  u'/Ucfl    OLD COFLOW PROFILE FROM PRELIMINARY RELEASE
    2.62     0.000   0.000      WAS FROM A DIFFERENT VERSION OF THE BURNER
    2.74     0.219   0.100      AS OPERATED AT SYDNEY UNIVERSITY.
    2.88     0.340   0.124
    2.90     0.370   0.130
    3.12     0.495   0.128
    3.62     0.660   0.101
    4.12     0.780   0.073
    4.62     0.850   0.053
    5.12     0.900   0.035
    5.62     0.940   0.021
    6.12     0.970   0.010
    6.62     0.990   0.010
    7.12     1.000   0.010
    40.0     1.000   0.010
```

MIXTURE FRACTION DEFINITION

Mixture fraction in the experimental results is defined following Bilger, except that only the elemental mass fractions of hydrogen and carbon are included. This is because the jet- and coflow boundary conditions for the elemental oxygen mass fraction are relatively close, and shot noise in the measurements of elemental oxygen mass fraction causes additional noise in the mixture fraction as normally defined. The mixture fraction based on C and H is tabulated in the data files. Averaged experimental results using the Bilger definition and the present modification do not differ significantly because differential diffusion effects are relatively small in these flames [4]. Calculations can use the normal definition of the Bilger mixture fraction, since the two will be identical unless the calculation includes differential diffusion.

$$F = \frac{0.5(YH-Y2H)/WTH + 2(YC-Y2C)/WTC}{0.5(Y1H-Y2H)/WTH + 2(Y1C-Y2C)/WTC}$$

where

```
    YH  = H element mass fraction in the measured sample
    YC  = C element mass fraction in the measured sample

    Y1H = H element mass fraction in main jet stream
    Y1C = C element mass fraction in main jet stream

    Y2H = H element mass fraction in coflow stream
    Y2C = C element mass fraction in coflow stream

and  WTH = 1.008, WTC = 12.011  are atomic weights.
```

The elemental mass fractions used in the data reduction process are listed below. Here the ambient humidity in the coflow air is included, and the composition of dry air is taken to be 21% O_2 and 79% N_2 (Ar and CO_2 content are neglected).

```
    Jet:     Y1H=0.0393, Y1C=0.1170, Y1O=0.1965, Y1N=0.6472

    Coflow:  Y2H=0.0007, Y2C=0.0000, Y2O=0.2413, Y2N=0.7580
```

The stoichiometric value of the mixture fraction is Fstoic=0.351

MEASUREMENT LOCATIONS AND GLOBAL PARAMETERS

The axial profiles of scalar measurement in the four flames includes locations x/d = 5, 10, 15,…,75 The radial profiles were obtained at x/d = 1, 2, 3, 7.5, 15, 30, 45, 60, and 75 in each flame.

The visible length is approximately:

```
Lvis ~ 67d (48 cm)
```

The stoichiometric flame length varies slightly for the four flames, based upon interpolation of the axial profile of Favre average mixture fraction as shown in Fig. 4. Values are:

```
Lstoic/d = 44.6, 47.0, 48.7, and 47.5 for flames C, D, E, and F.
```
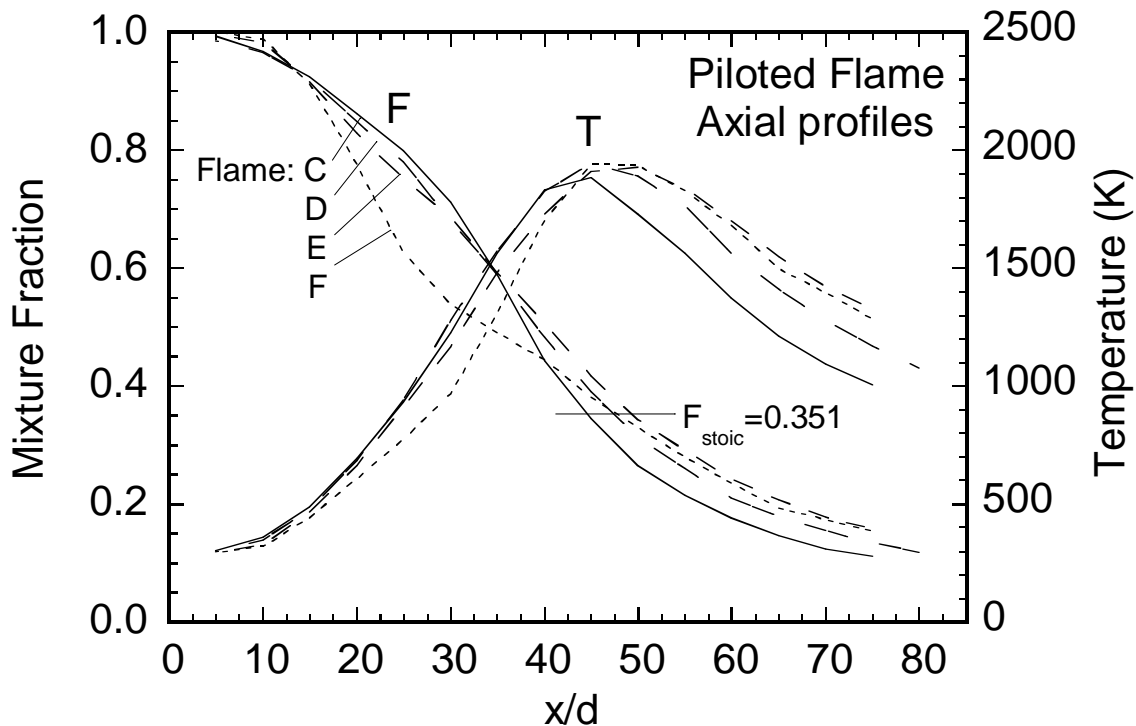

Fig. 4. Axial profiles of measured mixture fraction and temperature (Favre average) in piloted flames C, D, E, and F.

Total flame radiation was measured by Frank et al. [13], using a calibrated wide-angle, heat flux radiometer (Medtherm) with a ZnSe window.

```
Frad = 0.064, 0.051, 0.041, and 0.030 for flames C, D, E, and F.
```

AVAILABLE DATA AND FILE DESCRIPTIONS

There are two folders for each flame in the archive. The statistics (.stat) folder contains mean and rms scalar values bases on Favre (.Yfav), ensemble (.Yave), and conditional (.Ycnd) averages. The scatter (.scat) folder contains files of all single-shot results (.Yall) from each radial profile from x/d=7.5 on downstream. Radius is listed for each shot. All species data are reported as mass fractions. Files include column labels. The column labels and the data are separated by 1 or more spaces (not tabs). Example file names are:

```
File name     Description

DCL.Yfav    Flame D, axial (centerline) profile, Favre average mass fractions
E15.Ycnd    Flame E, conditional means, rms mass fractions at x/d=15
F45.Yall    Flame F, all single shot results from x/d=45
```

COMMENTS ON THE DATA

Temperatures are from Rayleigh scattering measurements, except in the radial profile at x/d=1, 2, and 3, where scattering from the burner caused the Rayleigh temperatures to be less reliable. Temperatures listed for x/d=1, 2, and 3 were determined from Raman/LIF total number densities, the measured ambient pressure, and the perfect gas law.

With a probe volume of 0.75 mm, spatial averaging effects are expected to be significant for scalar measurements in high-gradient regions near the flame base (x/d=1, 2, and 3).

The CO-LIF measurements should be used for comparisons with model predictions. CO mass fractions from Raman and LIF are included in the data archives. Differences are relatively small in the Favre and ensemble average profiles. However, the CO-Raman measurement is more strongly affected by hydrocarbon fluorescence interferences. Imperfect corrections of these interferences cause errors in the conditional means in the region of high interference on the fuel-rich side of the reaction zone.

Raman scattering measurements of CH_4 actually include signal from other hydrocarbon species that are formed in the flame. The high-temperature calibration used in processing these turbulent flame data was adjusted so as to yield a reasonable approximation of the total hydrocarbon mass fraction, based on measured and calculated profiles in laminar CH_4/air flames. As CH_4 concentration becomes small in these flames, the Raman signal increasingly corresponds to other hydrocarbon species. This is illustrated in Fig. 4, which shows conditional means of measured "CH_4" mass fraction (labeled as Y_{H-C} in the figure) along with calculated results (from TNF3), using PDF, CMC, and Monte-Carlo flamelet models. CH_4 and total hydrocarbon mass fractions, Y_{CH4} and Y_{H-C} are plotted for the PDF calculation. The conclusion is that differences between Y_{CH4} and Y_{H-C} are small compared to differences among the three predictions of Y_{CH4}.
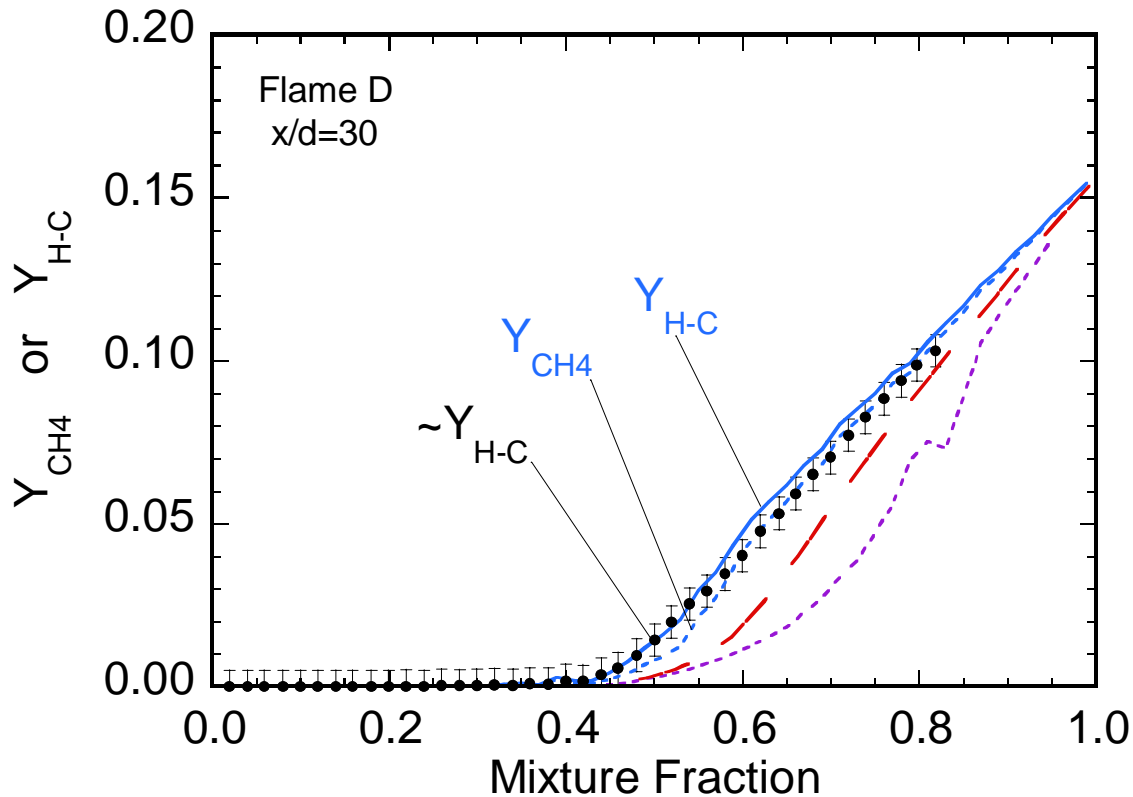
Fig. 4. Comparison of CH_4 and total hydrocarbon mass fractions in flame D.

COMMENTS ON COLLABORATIVE COMPARISONS

There has been much discussion in the TNF Workshops about the fact that flame F is very close to global extinction above the pilot flame and is consequently very sensitive to small changes in experimental conditions and model parameters. Modeling of the trends observed in the series of piloted flames is therefore considered more valuable than achieving a close match to the flame F results in isolation.

To facilitate useful comparisons of the details of scalar results from various calculations in the context of the TNF Workshop, we suggest the following. Some suggestions may be impractical for expensive calculations.

- Adjust the turbulence/mixing code to match the measured axial velocity profile and the stoichiometric flame length (Favre average), and report adjustments. Agreement within +/- 5% (if practical) on the stoichiometric flame length will ensure that no two predictions will differ by more than 10% in flame length. For some modeling approaches it may be necessary to adjust separate parameters to match both the velocity and mixture fraction profiles. Comparisons of detailed scalar results will be ambiguous, at best, if the overall flow and mixing fields are not in reasonable agreement.

- If NO is calculated, it would be useful to have both adiabatic and radiative calculations. Radiative calculations should use the approach documented on the TNF Workshop web

page (under Computational Submodels) and in Ref. [11]. More advanced calculations of radiation are welcome, and these will be most useful if parametrically compared with results from adiabatic and optically thin calculations.

- Comparisons are most informative if they are thorough. Past comparisons of these flames have included axial and radial profiles of mean and quantities and fluctuations, conditional mean and rms results, scatter plots of selected scalar (when available), and also derived scalars, such as the burning index.

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