Sandia/ETH-Zurich $CO/H_2/N_2$ Flame Data - Release 1.1

R. S. Barlow, G. J. Fiechtner, C. D. Carter, M. Flury

ABSTRACT

Scalar and velocity measurements on two turbulent nonpremixed jet flames of $CO/H_2/N_2$ fuel (40%/30%/30%) are described. Scalar measurements were conducted at Sandia National Laboratories, Livermore, California, using simultaneous Rayleigh/Raman scattering and laser-induced fluorescence to determine temperature and the concentrations of N_2, O_2, CO, H_2, CO_2, H_2O, OH, and NO. Velocity measurements were obtained at ETH Zurich, Switzerland, using a three-component laser-Doppler velocimetry system. These data are provided under the framework of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) to facilitate collaborative comparisons with results of calculations using various combustion models. The $CO/H_2/N_2$ jet flames retain the simple flow geometry of the hydrogen jet flames in the TNF data library, while adding a modest level of chemical kinetic complexity. The flames are attached and do not exhibit localized extinction. However, there is ample evidence of coupling between the time scales of flow and reaction. Therefore, these flames should serve as good test cases for submodels for mixing and the coupling of turbulence and chemistry.

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UPDATE HISTORY

15-DEC-98	First public release of the scalar and velocity data archives.
15-JAN-02	Update of references and inclusion of selected plots.

USE OF THE DATA

Please contact R. Barlow at the above address if you download or use these data. This will ensure that you will be on the mailing list for updates regarding these data and the activities of the TNF Workshop. Users are advised to check the web for updates to this data release and the included references.

Publications making use of these data should include the reference, R. S. Barlow et al., "Sandia/ETH-Zurich $CO/H_2/N_2$ Flame Data - Release 1.1," (2002), www.ca.sandia.gov/TNF, Sandia National Laboratories, as well as Refs. [1,7] listed below.

NOTICE

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

Experiments were conducted on two jet flames with different nozzle diameters but equal Reynolds numbers based on the cold jet exit conditions. The fuel composition for both flames was 40% CO, 30% H_2, 30% N_2 by volume. The nozzles were constructed from straight tubing with squared-off ends. The thick wall of the tubing allowed for a small recirculation zone that helped to stabilize the flames without a pilot. The flames were unconfined in all experiments. For the scalar measurements each burner tube was mounted such that the flame base was above the level of the 30-cm by 30-cm exit of the wind tunnel in Sandia's TDF laboratory. Both flames appeared to be fully attached to the nozzle, and there is no evidence in the data that oxygen is entrained into the fuel jet through extinguished zones near the nozzle.

In the scalar experiments, axial profiles were obtained in both flames and include measurements from x/d=20 to x/d=75 with steps of 5d. Radial profiles were obtained at axial positions of x/d=20, 30, 40, 50, and 60 in each flame. Measurements were not taken closer to the nozzle because we wished to avoid spatial averaging effects. The spatial resolution of the scalar measurements is ~0.75 mm. Typically, 800 to 1000 shots were collected at each location in these profiles. The data base includes Favre, Reynolds, and conditional statistics of both mass fractions and mole fractions. In addition, the complete files of single-shot mass fractions and mole fractions are available. Ref. [1] provides detailed discussion of the scalar results, including information on differential diffusion, partial equilibrium, mixture fraction pdf's, and the radial dependence of conditional means.

The three-component LDV measurements extend closer to the jet exit and include radial profiles at the exit and at x/d=10 in each flame. Tabulated velocity data in this archive are limited to velocity statistics and Reynolds stresses. Ref. [7] includes results and discussion on autocorrelations, energy spectra, wavelet analysis, and comparisons of the mixing structure of these $CO/H_2/N_2$ flames and the Sandia/ETH-Zurich H_2/He flames, which are also documented in the TNF data archives.

BOUNDARY CONDITIONS

Nozzle dimensions and bulk jet exit velocities are listed in Table 1. The elemental mass fractions in the fuel and air streams, as they were specified in the data reduction process, are listed in Table 2.

Table 1 Nozzle Dimensions and Flow Conditions*

Flame	d, Nozzle ID (mm)	Nozzle OD (mm)	U_{jet} (m/s)	Re_{jet}
A	4.58	6.34	76.0 ± 1.5	~16,700
B	7.72	9.46	45.0 ± 0.9	~16,700

* $Re=U_{jet}d/\nu$, where ν=2.083x10^{-5} m^2/s

Table 2 Elemental Mass Fraction Boundary Conditions*

Stream	Y_C	Y_H	Y_O
Fuel, 1	0.2377	0.0299	0.3167
Coflow, 2	0.0	7.7x10^{-4}	0.2356

* Coflow humidity included, CO_2 content in air neglected, balance is N_2.

The coflow air conditions for the scalar experiments at Sandia were 0.75 m/s ± 0.05 m/s velocity, 290 K ± 2 K temperature, and 0.012 ± 0.002 mole fraction of H_2O vapor. Coflow velocity for the LDV measurements at ETH-Zurich was 0.65 m/s. We suggest that calculations be performed with a coflow velocity of 0.70 m/s, but it should not be necessary to repeat calculations performed with either 0.65 or 0.75 m/s coflow. The jet exit temperature was 292 K ± 2 K. Jet flow boundary conditions may be taken from the measured profiles at x/d=0, which should approximate fully developed turbulent pipe flow.

EXPERIMENTAL METHODS AND MEASUREMENT UNCERTAINTIES

Multiscalar experiments were conducted in the Turbulent Diffusion Flame (TDF) laboratory at Sandia's Combustion Research Facility. The flow facility, diagnostic systems, and calibration procedures are described in Refs. [1-4]. The combination of spontaneous Raman scattering and Rayleigh scattering was used to measure the major species concentrations (N_2, O_2, CO, H_2, CO_2, H_2O) and temperature. Linear LIF was used to measure the concentrations of OH and NO. Fluorescence signals were corrected on a shot-to-shot basis for variations in the Boltzmann fraction and collisional quenching rate, based on measured temperature and major species concentrations in the probe volume. Collisional quenching cross sections for OH and NO were based on the work of Paul et al. [5,6].

The precision of the scalar measurements is represented Fig. 1, which shows results of processed data from a series of CO/H_2-air flat flames (50/50 fuel mixture) operated on a Hencken burner (uncooled, nonpremixed matrix burner). The symbols show mean temperature and species mole fractions from each operating condition of the burner, and each symbol is surrounded by an ellipse having major and minor axes of twice the standard deviations (±σ) of the scalar and the mixture fraction. The standard deviations in these calibrations may be used to estimate the contribution of random error (primarily shot noise) to the conditional fluctuations reported in this data archive. Representative values of precision are listed in Table 3 for specific flame conditions.

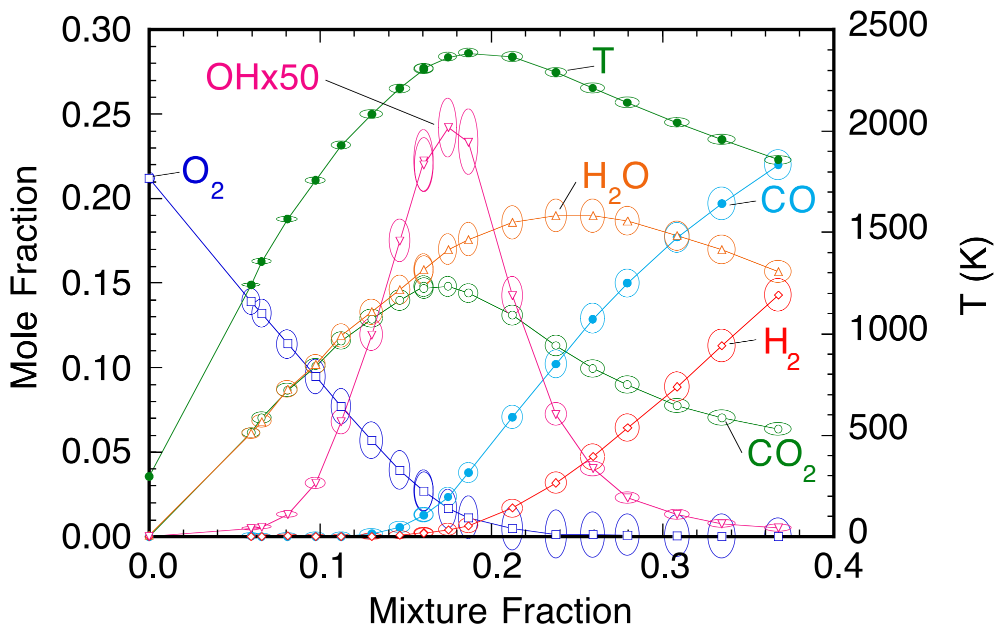

Fig. 1. Measured temperature and species mole fractions in the product gases above a series of CO/H_2-air calibration flames stabilized on a Hencken burner. Symbols show mean values from the Raman/Rayleigh/LIF data reduction process. Ellipses show standard deviations (±σ) of the measured scalars and the calculated mixture fraction.

Estimates of systematic uncertainties (absolute accuracy of averaged values) are also listed in Table 3 and are based on analysis of the calibration methods, repeatability of calibrations, considerations of calibration drift, allowances for greater uncertainties within the interpolated regions (approx. 900K to 1600K) of the calibration curves for H_2 and CO, and uncertainties in gas flow rates. Flow controllers were calibrated using laminar flow elements, and these calibrations were repeatable to within ±1%. The estimated uncertainties in averaged temperature and concentration measurements are illustrated in Fig. 2. Here, averaged results are plotted versus the equivalence ratio for 18 CO/H_2-air flame conditions. The lower values from Table 1 are plotted as error bars. Where no error bars are visible the uncertainty is represented approximately by the size of the plotting symbol. The solid curves in Fig. 2 show results of non-adiabatic equilibrium calculations computed at temperatures representing the average Rayleigh temperature from several calibration sets. These averaged Rayleigh temperatures are about 50K below adiabatic in these calibration flames. The OH calibration is based on independent laser absorption measurements in a CH_4-air flame, and this is consistent with the calculated non-adiabatic equilibrium OH levels in the CO/H_2-air flames, as shown in Fig. 2.

Table 3 Relative standard deviations of scalars measured in flat flames and estimated systematic uncertainties

Scalar	σ(rms)	Conditions (mass fraction, T)	Systematic Uncertainty
T	1%	2140 K[a]	2%
Y_{N2}	2%	0.73, 2140 K[a]	3%
Y_{H2O}	5%	0.12, 2140 K[a]	3-5%
Y_{CO2}	6%	0.14, 2140 K[a]	3-5%
Y_{CO}	13%	0.062, 2020 K[b]	5-10%
Y_{H2}	17%	0.003, 2020 K[b]	5-10%
Y_{OH}	8%	0.0016, 2140 K[a]	10%
Y_{NO}	10%	8 ppm, 1760 K[c]	10-15%

[a] Premixed CH_4/air, ϕ=0.96, uncooled (Hencken) burner

[b] Premixed CH_4/air, ϕ=1.27, uncooled (Hencken) burner

[c] Premixed $CH_4/O_2/N_2$, ϕ=0.72, cooled (McKenna) burner

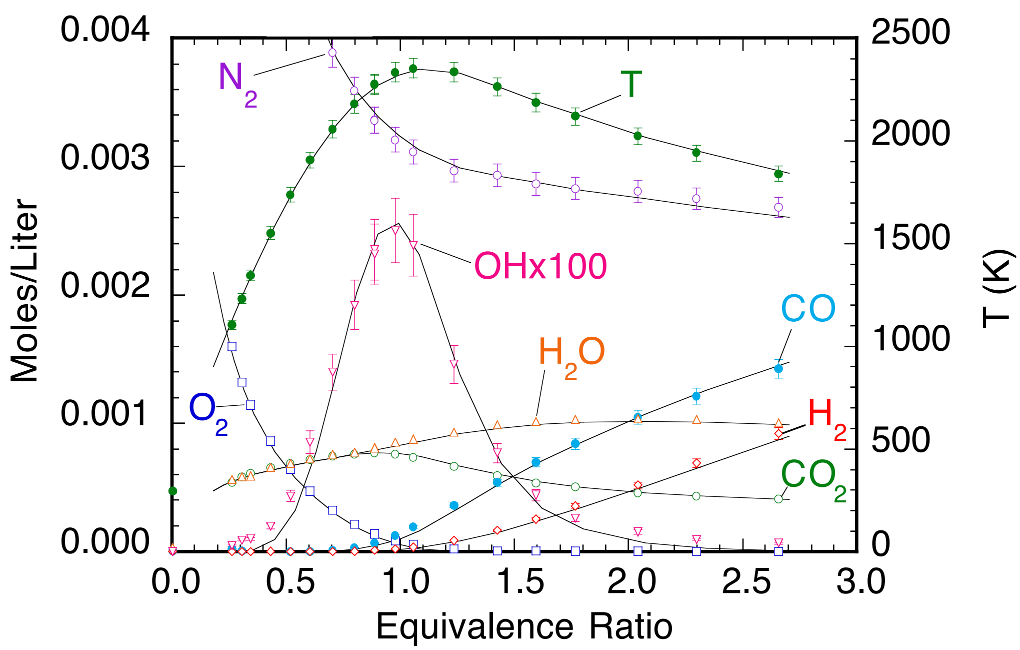

Fig. 2. Processed mean values of temperature and concentration in the CO/H_2-air Hencken-burner flames. Error bars show estimated uncertainties, as listed in Table 3 (lower values). Solid lines connect non-adiabatic equilibrium values calculated at the measured Rayleigh temperatures.

Velocities were measured at ETH Zurich, using a Dantec 3-component (three color) LDV system. Details of the measurements are described in Ref. [7]. Air and fuel streams were seeded, and the Shannon algorithm [8] was used in reconstructing the velocity data.

FILE NAMES AND FORMATS

Scalar data file names use the following system to indicate the flame, location, and type of data in the file. There are three types of averaged data files and two types of files that include single shot data. Scalar data files are in ASCII format with columns separated by one or more spaces.

Example scalar file name: chnAd20Y.ave

Flame case chnA or chnB:
- chnA
- chnB

Location:

d20	x/d=20, radial profile
d30	x/d=30, radial profile
d40	x/d=40, radial profile
d50	x/d=50, radial profile
d60	x/d=60, radial profile
cl	centerline or axial profile (no conditional mean results)

Data type (mass fraction or mole fraction):

Y	mass fraction
X	mole fraction

File extension

.ave	radial profile of ensemble averages (mean and rms)
.fav	radial profile of Favre averages (mean and rms)
.cnd	conditional averages (mean and rms) of all data at that axial location
.all	all single-shot results from a radial profile with radius (mm) tabulated

Column labels are included in all files. The statistical data files include radial or axial location in mm and the mean and rms values of Fblgr, T, O_2, N_2, H_2, H_2O, CO, CO_2, OH, NO, and TNDR.

Mixture fraction is defined following Bilger as:

$$F_{b\lg r} = \frac{2(Y_C - Y_{C,2})/w_C + (Y_H - Y_{H,2})/2w_H - (Y_O - Y_{O,2})/w_O}{2(Y_{C,1} - Y_{C,2})/w_C + (Y_{H,1} - Y_{H,2})/2w_H - (Y_{O,1} - Y_{O,2})/w_O}$$

where Y's are elemental mass fractions of carbon, hydrogen, and oxygen; w's are atomic weights; and the subscripts 1 and 2 refer to the fuel stream and coflowing air stream, respectively. The fuel and air boundary conditions for the elemental mass fractions are listed in Table 2. The stoichiometric value of the mixture fraction is 0.295 in these flames.

TNDR is defined as the ratio of total number densities determined from Raman/LIF and Rayleigh measurements. Equivalently, TNDR is equal to the ratio of temperatures determined from Rayleigh and Raman measurements.

TNDR = (Raman/LIF Number Density)/(Rayleigh Number Density)

TNDR = (Rayleigh temperature)/(Perfect Gas Temperature from Raman-LIF data)

In these measurements the temperature determined from Rayleigh scattering is tabulated and is considered to be more accurate than the temperature determined using the perfect gas law and the total number density of measured species. TNDR is tabulated with the single-shot data to allow the original species concentrations to be recovered from the mass fractions. Shot noise will cause TNDR to differ from unity for single-shot measurements. Calibration uncertainties can also cause TNDR to differ from unity in single-shot and averaged results. Ensemble-average and conditional-average results for TNDR are tabulated in the .ave and .cnd files. For most files the average value of TNDR is within a few percent of unity.

Velocity data files are in ASCII format with columns separated by tabs. File names have the form seqDDdd.dat, where DD refers to the diameter of the tube and dd refers to location of the profile.

Flame Case (DD):

14	flame chnA, 1/4-inch diameter tube
38	flame chnB, 3/8-inch diameter tube

Profile location (dd):

00	radial profile at jet exit
10	radial profile at x/d=10
20	radial profile at x/d=20
30	radial profile at x/d=30
40	radial profile at x/d=40
50	radial profile at x/d=50
60	radial profile at x/d=60
ax	axial profile

The coordinate system for the LDV data files is x,y,z, with z being the axial coordinate and x being the direction of radial traverse. Velocity components are labeled as ux, uy, and uz. Files include: x, y, z, ux, rmsux, uy, rmsuy, uz, rmsuz, uxuz, uzuy, uxuy. These designate location in mm, mean velocities and rms fluctuation in m/s, and Reynolds shear stresses in m^2/s^2.

ACKNOWLEDGMENTS

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REFERENCES

1. Barlow, R. S., Fiechtner, G. J., Carter, C. D., and Chen, J.-Y., "Experiments on the Scalar Structure of Turbulent $CO/H_2/N_2$ Jet Flames," *Combust. Flame* 120:549-569 (2000).
2. Nguyen, Q. V., Dibble, R. W., Carter, C. D., Fiechtner, G. J., and Barlow, R. S., *Combust. Flame* 105:499-510 (1996).
3. Barlow, R. S., Fiechtner, G. J., and Chen, J.-Y., *Twenty-Sixth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1996, pp. 2199-2205.
4. Barlow, R. S., and Frank, J. H., *Twenty-Seventh Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1998 (in press).
5. Paul, P. H., *JQSRT* 51:511-524 (1994).
6. Paul, P. H., Gray, J. A., Durant Jr., J. L., and Thoman Jr., J. W., *AIAA J.* 32:1670-1675 (1994).
7. Flury, M., "Experimentelle Analyse der Mischungstruktur in turbulenten nicht vorgemischten Flammen," Ph.D. Thesis, ETH Zurich, Switzerland (1998).
8. Veynante, D. and Candel, S., *Exp. Fluids* 6:534-540 (1988).

APPENDIX: SELECTED PLOTS OF SCALAR RESULTS FOR CO/H2/N2 JET FLAMES

List of Figures:

Axial Profiles of Favre Mean and RMS Scalars

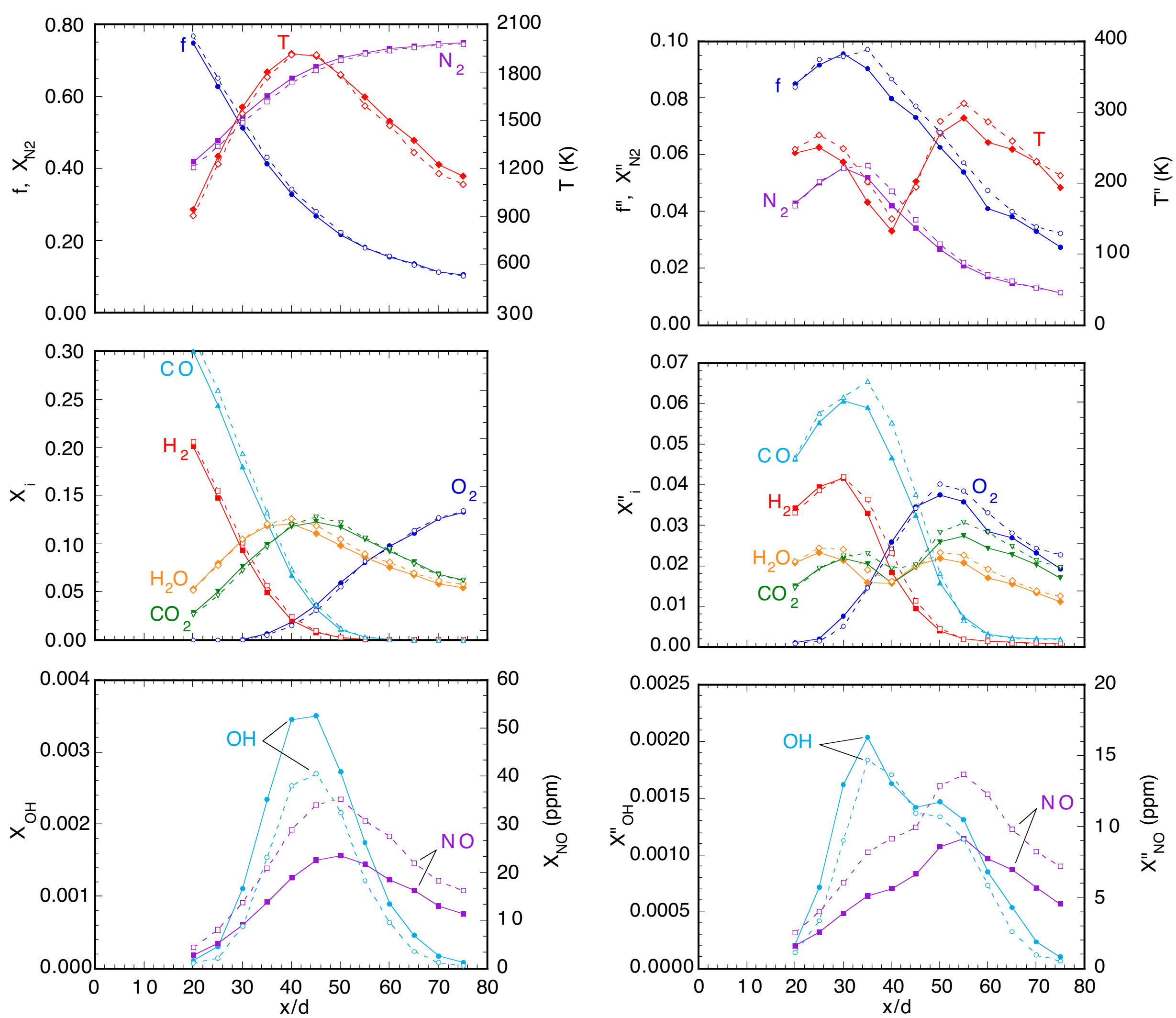

Fig. A1. Axial profiles of Favre average mixture fraction, temperature and species mole fractions are shown in the three graphs on the left for flames chnA (solid lines) and chnB (dashed lines). Axial profiles of scalar fluctuations are plotted on the right. Axial distance is scaled by the jet exit diameter for each flame.

Radial Profiles of Favre Average Scalars at x/d=20 and x/d=50

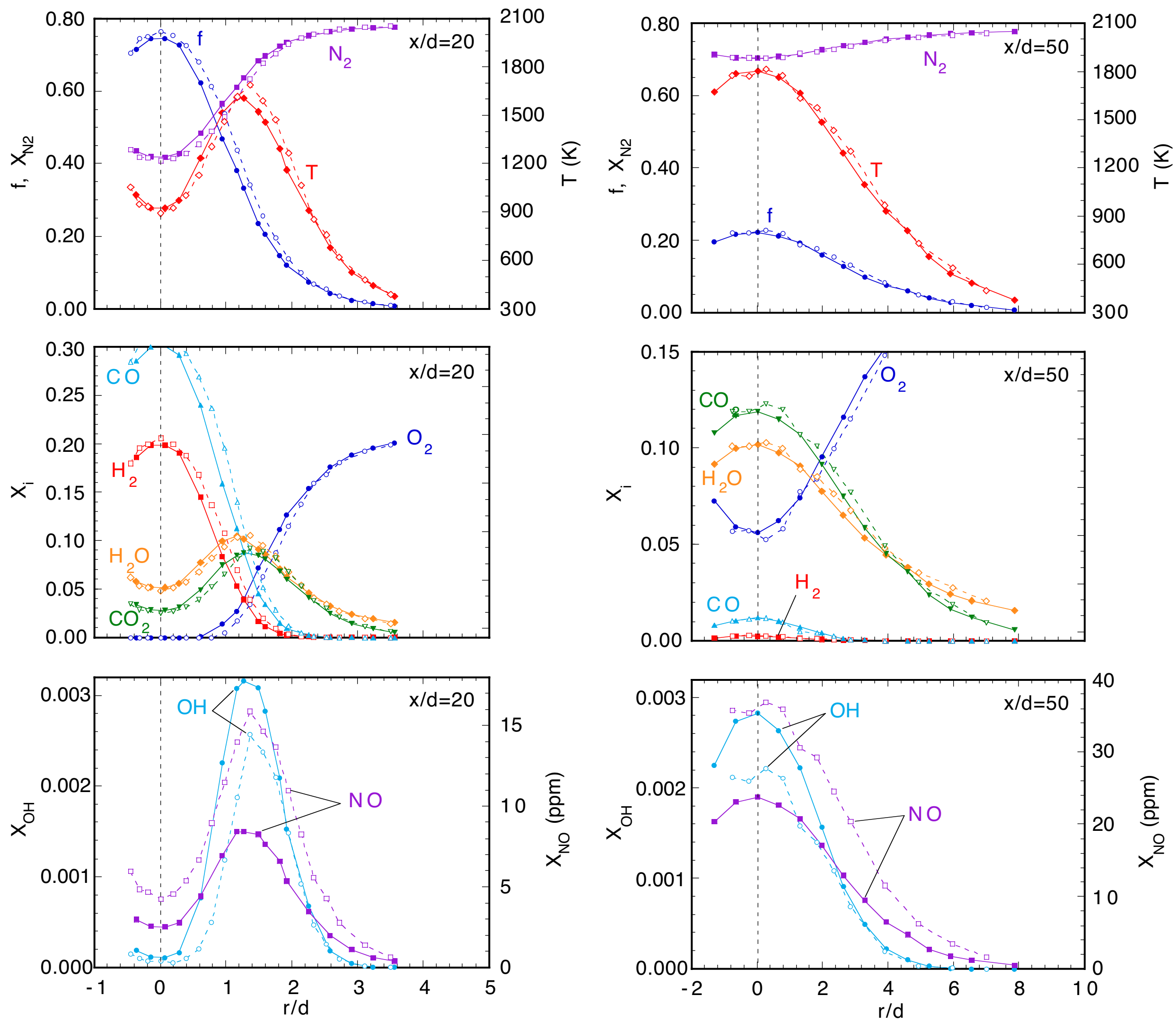

Fig. A2. Radial profiles of Favre averaged scalars in the two flames, A (solid lines) and B (dashed lines), measured at axial locations x/d=20 (left) and x/d=50 (right). The Favre average stoichiometric flame length is about 47d in both flames.

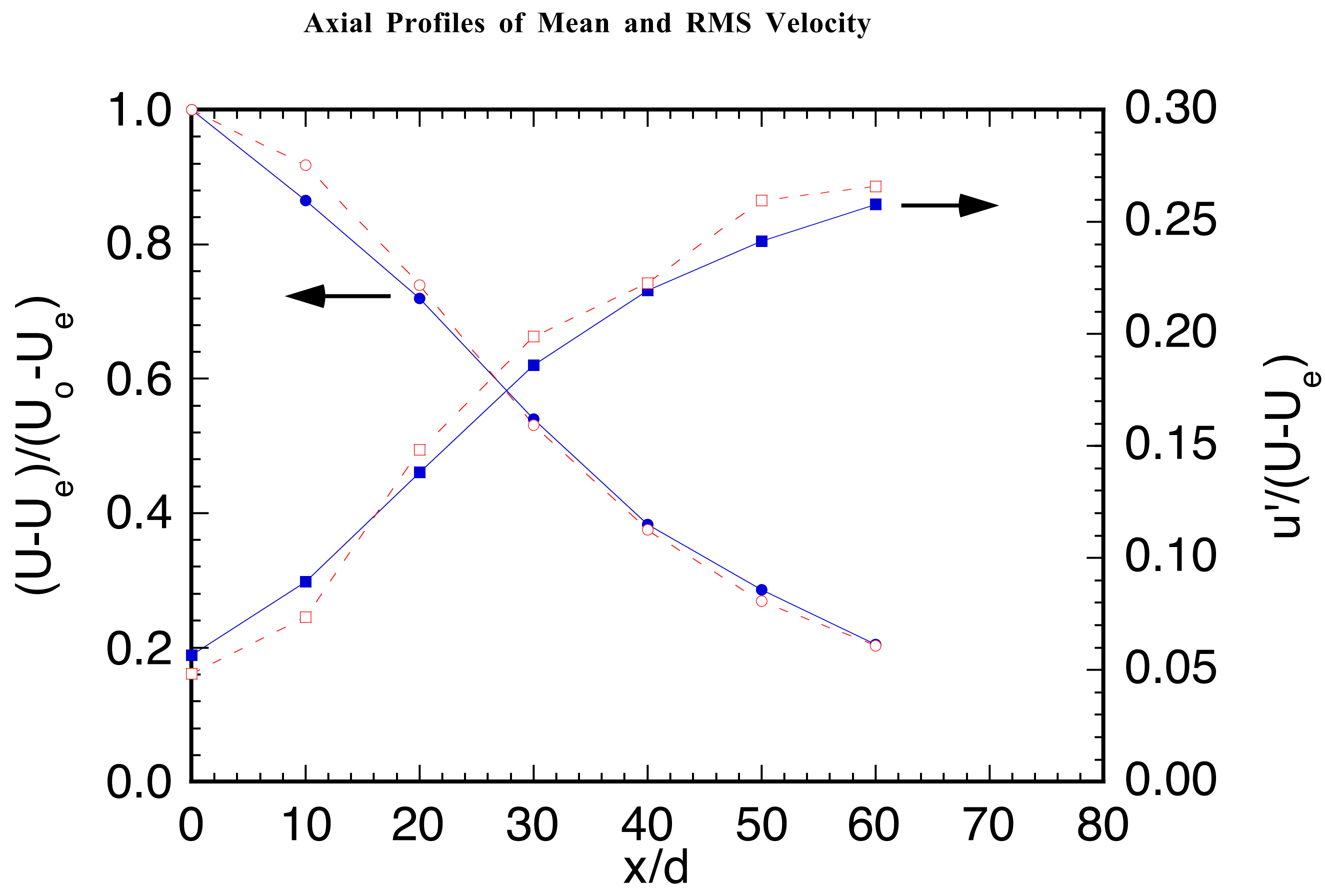

Fig. A3 Axial profiles of mean and fluctuating velocity from LDA measurements by M. Flury for flames chnA (solid lines) and chnB (dashed lines). Ue is the coflow velocity, and Uc is the nozzle exit velocity on the centerline.

Radial Profiles of Mean and RMS Velocity at x/d=20 and x/d=50

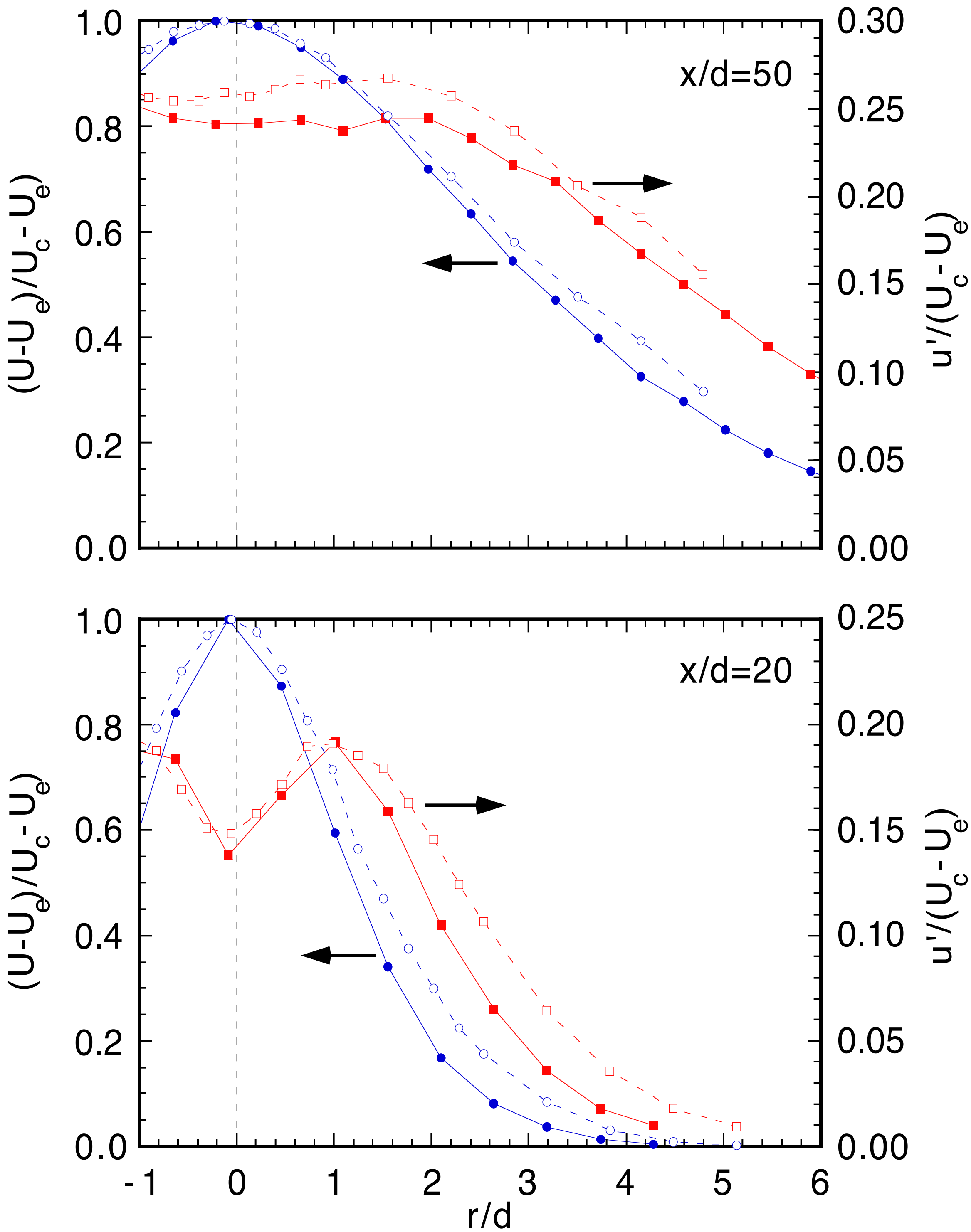

Fig. A4 Radial profiles of mean and fluctuating axial velocity from LDA measurements by M. Flury for flames chnA (solid lines) and chnB (dashed lines) at x/d=20 (lower graph) and x/d=50 (upper graph). Ue is the coflow velocity, and Uc is the nozzle exit velocity on the centerline.

Scatter Plot of Temperature and O_2 Mole Fraction in Flame chnA at x/d=20

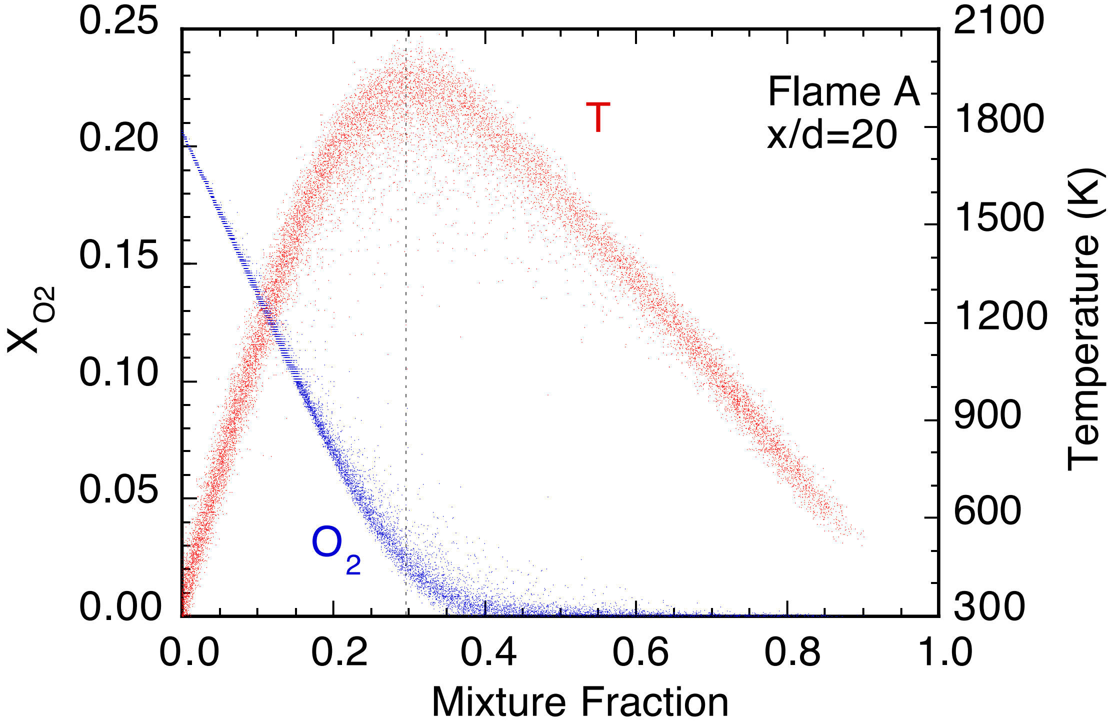

Fig. A5 Scatter plot of single-shot temperature and O_2 measurements in flame chnA at x/d=20, including approximately 15,000 samples from the complete radial profile. The vertical dashed line indicates the stoichiometric value of the mixture fraction. This is the most highly strained location for the scalar measurements in this data set.

Conditional Mean and RMS Fluctuation of Temperature and O_2 Mole Fraction in Flame chnA at x/d=20

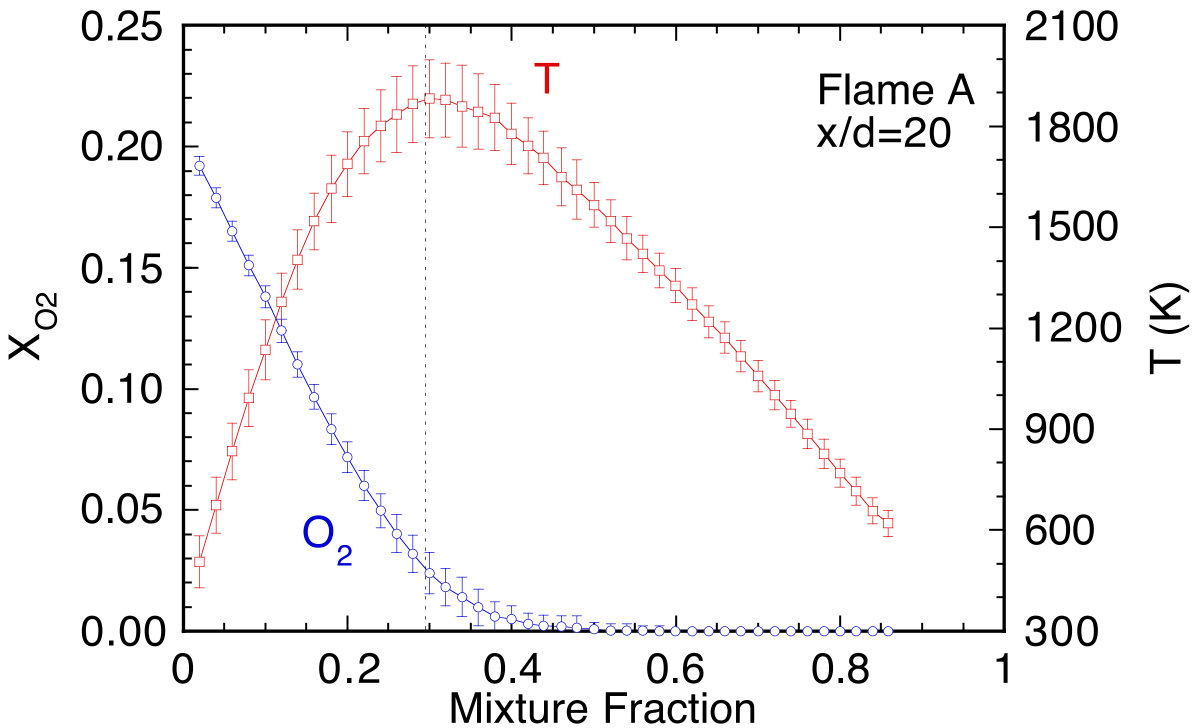

Fig. A6 Conditional mean and rms fluctuation (plotted as uncertainty bars) calculated from the data of shown above for flame chnA at x/d=20, using evenly-spaced intervals of 0.02 in mixture fraction. The vertical dashed line indicates the stoichiometric value of the mixture fraction.

Measured Conditional Means Compared with Strained Laminar Flame Calculations

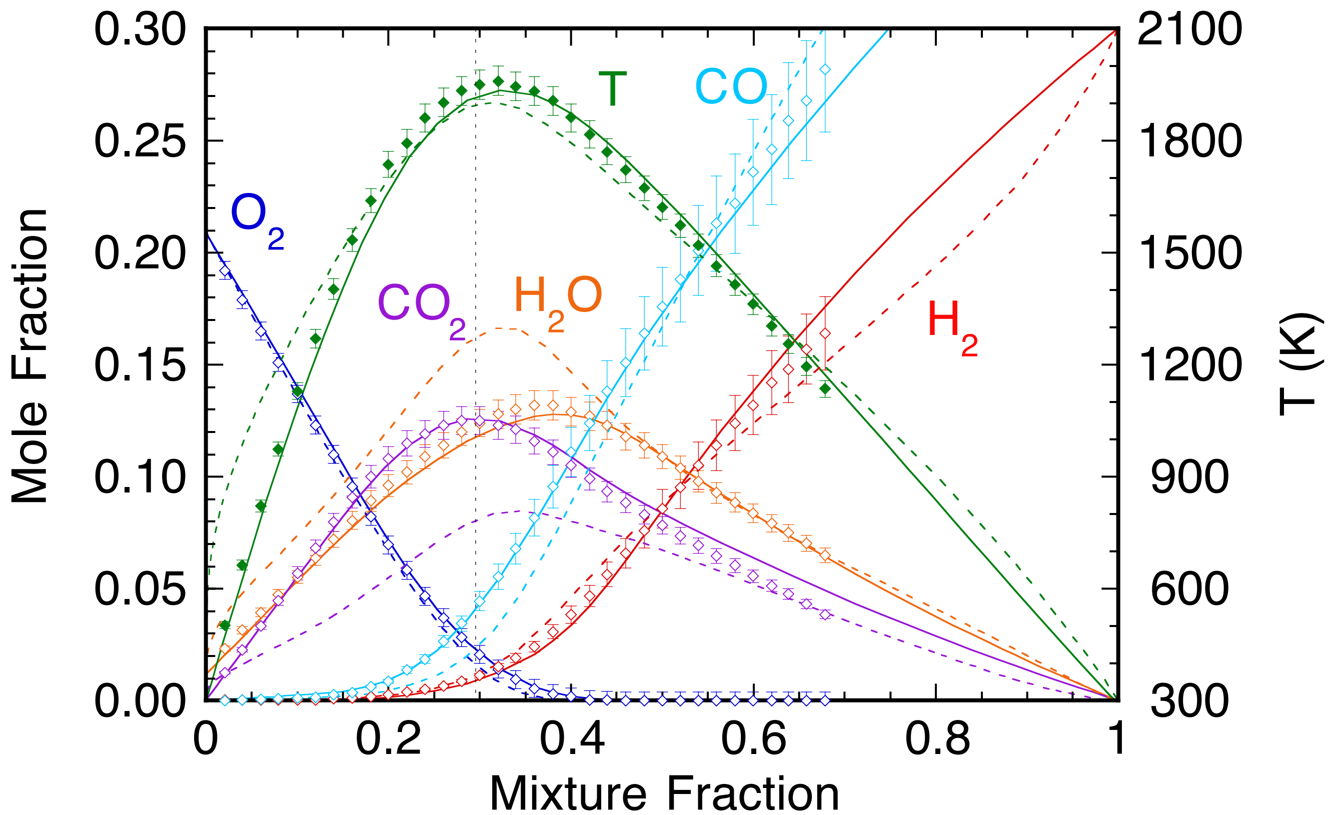

Fig. A7. Measured conditional means at x/d=30 in flame chnA compared with the two types of laminar calculations: full transport (dash lines) and equal diffusivities (solid lines). Estimated experimental uncertainties are plotted as the larger values in Table 3 of the documentation file (Table 1 of the paper). The calculation with equal diffusivities yeilds a better approximation of the turbulent flame data. The vertical dashed line indicates the stoichiometric value of the mixture fraction.

Measured Conditional Means of CO and CO_2 Compared with Strained Laminar Flame Calculations

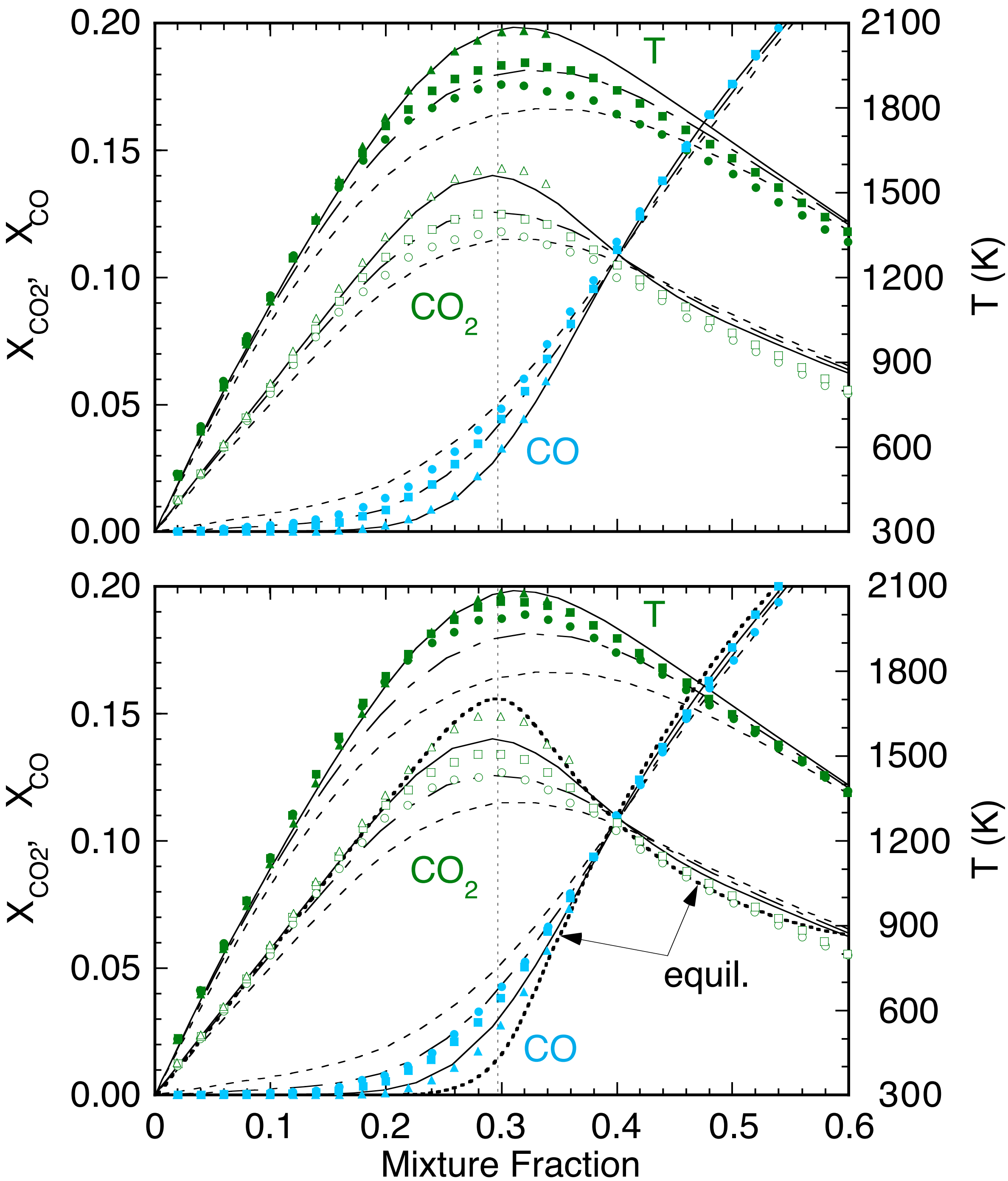

Fig. A8. Conditional means of XCO_2, XCO, and T in flames chnA (upper) and chnB (lower) at streamwise locations x/d=20 (circles), x/d=30 (squares), and x/d=50 (triangles). Curves are plotted for the equal-diffusivity flame calculations at strain rates of $a=10\ s^{-1}$ (solid), $a=100\ s^{-1}$ (chain-dash), and $a=400\ s^{-1}$ (dash). Adiabatic equilibrium curves (short dash) for XCO_2 and XCO are included in the lower graph.