# Proceedings of the 2nd International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

Heppenheim, Germany

June 3–4, 1997

Edited by
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Organizing Committee: R. Barlow, R. Bilger, J.-Y. Chen, E. Hassel, J. Janicka, A. Masri, N. Peters

**Abstract**

This report gives a summary of the 2nd International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames, which took place in Heppenheim, Germany on June 3-4, 1997. The first part tries to collect the important findings of the workshop whereas the second part consists of some of the material that was presented at the workshop and handed out to the organizers.

A total of 53 people participated in the workshop. In the two-day program the scientists a) resembled the data concerning the simpe hydrogen jet flames, b) discussed relevant issues concerning measurement and computation of methane flames and c) made decisions on future standard flames.

The organizers again wish to express their thanks to the sponsors of this workshop as there were the companies of Coherent, Spectroscopy & Imaging, Cray Research, TSI, Spectra Physics, Dantec/invent.

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| 50 | Wolff | Dr. | Dagmar | University of Stuttgart | |
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| 52 | Xiao | Mr. | Kejian | University of Stuttgart | |
| 53 | Zhang | Dr. | Y. | UMIST, Dept. of Mech. Eng. | YZ100@umist.ac.uk |

# 2 Agenda

## Monday 2 June,

**18:20** Guided village tour in English around Heppenheim, meeting point: main entrance **RAMADA HOTEL**

## Tuesday 3 June

**8:00 - 9:00** Registration at the Kurfürstensaal, set up posters

**9:00** Welcome, introduction, agenda, scientific content, announcements
(President of TH Darmstadt, Janicka, Hassel)

**9:30** Summary of Naples workshop, Web status, and activities since Naples (Barlow - 15 min, plus 15 minutes for discussion)

**10:00** $H_2$ flames: Comparison of turbulence fields
(J. Janicka - Moderator)
(Pfuderer (THD) - 15 min, plus 15 minutes to begin discussions)

**10:30** Coffee and Posters

**10:45** H2 flames: Comparison of scalar fields, including NO
(E. Hassel - Moderator)
(Chen - 20 min, plus 40 min for discussion)

**12:00** Lunch and Posters

**13:30** Continued discussion of H2 flames and other special topics
(R. Barlow - Moderator)
(Accuracy of radiation measurements and models: Gore - 15 min)
(Transient flamelets: Peters - 15 min)
(Unresolved issues in H2 flames, priorities for future work)

**15:00** Coffee and Posters

**15:15** Methane flames: Status of piloted flame data sets and calculations
(J-Y Chen - Moderator)

**16:45** Coffee, posters, small group discussion

**19.00** Dinner with wine tasting in Heppenheim

## Wednesday 4 June

**9:00** Methane flames: Definition of model problem(s) for Boulder
(S. Pope - Moderator)
(Action items and schedule to get all necessary data, submodels, and guidelines onto the Web)

**10:30** Coffee and Posters

**10:45** Continued discussions of methane flames, possible small group discussions

**12:15** Lunch and posters

**13:30** Final Discussions
(Janicka/Hassel/NN - Moderator)
(Funding perspectives, publication possibilities, future research priorities and organization of the Boulder workshop)

**15:00** Coffee and posters

**16:00** Transfer to the Technical University of Darmstadt for laboratory tour
(Please make your registration at the registration desk)

## Sponsoring Companies

**Coherent GmbH**
Dieselstr. 5b
64807 Dieburg
Tel.: 06071 968 0

**Spektroscopy&Imaging**
Schlehengrund 16
59597 Erwitte
Tel.: 02943 2041

**Cray Research Unit**
Am Hochacker 3
85630 Grasbrunn-Neukeferloh
Tel.: 089 46108 0

**TSI GmbH**
Ziegelerstr. 1
52078 Aachen
Tel.: 0241 52303 0

**Spectra Physics GmbH**
Postfach 101351
64213 Darmstadt
Tel.: 06151 708 0

**Dantec/invent**
Measurement Tech. GmbH
Am Weichselgarten 21
91058 Erlangen
Tel.: 09131 7776 0

# 3 Experimental and Modeling Issues

### Hydrogen Flames

Turbulence Model:

It is widely accepted that the turbulence model needs to be adapted to the problem in order to get accurate results. But, in any case, all changes are to be carefully documented. Modeling of the Reynolds stress tensor might be improved.

Mixing Models:

The distribution of mixture fraction is captured by all models (statistical, Euler– and Monte-Carlo–pdf).

Differential Diffusion:

Differential diffusion effects are visible e.g. in the OH distribution.

Measurement of OH and NO:

These measurements and computations need to be reexamined, they show large deviations.

### Methane Flames

Stabilization:

Several methods may be applied to stabilize the flame: pilot, bluff body, swirl, preheating, ...

Mixing Models:

IEM, EMST, CMC

# 4 Preparations for Boulder

Steven Pope kindly agreed to take part in the organization of the workshop and will be an additional member of the organizing committee.

### Proposed flames

The following methane flames were selected by the participants of the workshop as standard flames for the next workshop in Boulder.

1. Sydney piloted flame: velocity and scalars measured

2. Sandia piloted jet flame: 1/3 CH4/Air
3. $CO/H_2$ jet flame measured at Sandia/ETH Zürich
4. Delft piloted flame

### Time schedule

The next workshop will take place in Boulder, CO on July 31 – August 1, 1998. Each group associated with a standard flame is responsible for setting the format and collecting the data from modellers. Results are to be submitted two months ahead of the workshop.

### Publication of results

Publication of the results for the hydrogen flames is desired. The workshop organizers will look into the possibility of setting up a review article or presenting the results as invited lecture at the next combustion symposium.

## Copies of slides presented at the workshop

The remaining pages show copies of most of the slides that were presented at the workshop.

# Selected Slides from TNF2 Presentations and Discussions

- Most of the slides selected for inclusion here are concerned with comparisons of measured and modeled results for $H_2$ jet flames.
- We have not included presentations on hydrocarbon flames or on preparations for TNF3, as these topics are better documented on the web page and in the TNF3 Proceedings.
- Slides are presented roughly in the order of the agenda.
- Most slides were scanned from hard copies collected at the end of the workshop.
- Much of the work on comparisons of measured and modeled results in $H_2$ jet flames has been published, and interested readers are encouraged to consult the Bibliography on the TNF web site at http://www.ca.sandia.gov/TNF

*2nd Workshop on Measurement and Computation of Turbulent Nonpremixed Flames*

# *Measurements and Computations of EKT- Flame (H3) and Sandia/ETHZ -Flame ($H_2$He20)*

## Topic:

## *Velocity, Scalar and Temperature Fields, Turbulence Modeling Aspects*

the presented data is provided by:

**R. Barlow, Sandia (USA)**
**J.-Y. Chen, Berkeley (USA)**
**H. Sanders, CNRS-Orleans (France)**
**J. Ferreira, M. Flury and M. Schlatter, ETH Zürich (Switzerland)**
**W. Meier, S. Prucker, DLR-Stuttgart (Germany)**
**D. Pfuderer, M. Tacke, G. Früchtel,**
**E. Hassel, J. Janicka, EKT Darmstadt (Germany)**

**THANK YOU FOR YOUR COOPERATION !**

# Configurations and Experimental Data

## H3-Flame:

**setup:** D=8.0 mm, U0=34.8 m/s, Re=10.000, free

**fuel:** H2/N2 50/50 mole fraction

**data used:**
- <u>, <u''u''>, <v''v''>, <w''w''>, <u''v''> from LDV by *G. Früchtel*, EKT Darmstadt
- mixture fraction, temperature and major species from RAMAN/Rayleigh by *M. Tacke* and *S. Linow*, EKT Darmstadt and *W. Meier* and *S. Prucker*, DLR-Stuttgart

## H2He-Flame:

**setup:** D=3.75 mm, U0=294 m/s, Re=10.000, enclosed

**fuel:** H2/He 80/20 mole fraction

**data used:**
- <u>, <u''u''>, <v''v''>, <u''v''> from LDV by *J. Ferreira, M. Flury* and *M. Schlatter*, ETH Zürich
- mixture fraction, temperature and major species from RAMAN by *R. Barlow*, Sandia

# Comparison of Flame Computations (coarse overview)

| | Chen | Sanders | ETHZ | EKT | EKT |
|---|---|---|---|---|---|
| **H3** | x | x | | x | x |
| **H2He20** | x | | x | x | x |
| **turbulence model** | RSM Lumley (version ?) | RSM GL-IP | standard k-ε | standard k-ε | RSM JM (rev.) |
| calibration or modification | H3: no H2He: yes | $C_1$ =2.3 for cold jet | Pope's $C_{\varepsilon 2}$ -correction | H3: no H2He: $C_{\varepsilon 2}$=1.83 | H3: no H2He: $C_{\varepsilon 2}$=1.80 |
| **$\overline{\rho' u'}$-correlation** | no | yes | no | no | yes |
| **scalar model** | PDF | SMC: GL $\varepsilon_f$-equation ? | eddy diffus. (r=const.) | eddy diffus. r=0.5 | SMC: JM r=0.5 |
| calibration or modification | no | no | no | no | no |
| **chemistry model** | 5 step mechanism | flamelets / equilibrium | PEUL / (flamelets) | equilibrium | equilibrium |
| **coupling model** | PDF | β-function | (β-function) | β-function | β-function |
| **numerical scheme** | parabolic GEMIX | parabolic | elliptic | parabolic GENMIX | parabolic GENMIX |
| **computational cost** | 1,5 days on Pent. 200 | 5 min on DEC Alpha | ~ 12 h on HP | ~ 5 min. on Pent. 133 | ~ 5 min. on Pent. 133 |

ETHZ: ***J. Ferreira, M. Schlatter and M. Flury*** EKT: ***D. Pfuderer***

Dirk Pfuderer
E. Hassel & J. Janicka

# How to choose the *right* turbulence model ?

## 1.) use a standard model

**-But where is the standard model defined ?**
**-Especially for reacting flows there is a large variety of sub-model combinations and revised constants !**

⇒ ***The workshop may define a (some) standard model(s) !***

## 2.) use a *flow type* calibrated model

**A frequently supposed way is:**

| | |
|---|---|
| **1st step:** | **Calibrate the model on a cold air/air jet.** |
| **2nd step:** | **Formulate a model for nonreacting jets with density variations (He, $CH_4$ or $CO_2$ jets).** |
| **3rd step:** | **Use this model for flame calculations.** |

⇒ ***This approach fails !***

## 3.) use a calibration based on particular measurements

**-This is -more or less- always done !**
**-Needed to have a good overall accuracy !**
**-For the jet diffusion flames the *right way* might be:**

***„Take mean velocity measurements of the desired flow and calibrate $C_{\varepsilon 2}$ to meet the overall decay and spreading "***

**This only possible since the flow has a certain global development !**

# Results

a) **The two flames show different velocity field developments !**

**H3: -The standard k-ε and RSM models work quite well.**
**-Models calibrated to cold round jet spreading lead to a slower spreading of the mean fields and hence to longer flames.**

**H2He2: -All models need a correction to describe the decay of this flow and hence the correct flame length.**

b) **Mixture fraction: Statistical models, Euler- and Monte-Carlo pdf's show nearly identical results.**

c) **The major species and temperature are near equilibrium in both flames.**

**-5 step chemistry = equilibrium chemistry**
**-Due to differential diffusion in the laminar pre-calculations flamelets yield higher temperatures.**

d) **Proposal for a *standard* model for code testing and beginners:**
**(*concerning the calculation of H3 and H2HeXX*)**

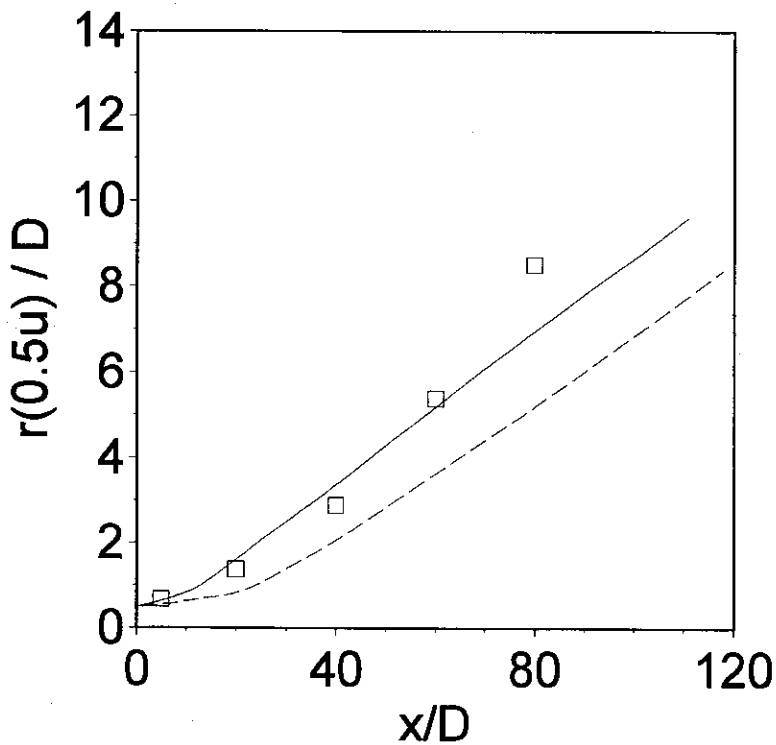
**Model A)** **k-ε-model (without extra terms), constant time scale ratio, beta function, equilibrium chemistry**
**($C_{\varepsilon 2}$ = 1.92 for H3, $C_{\varepsilon 2}$ =1.83 for H2HeXX, $\sigma_f$=? etc.)**

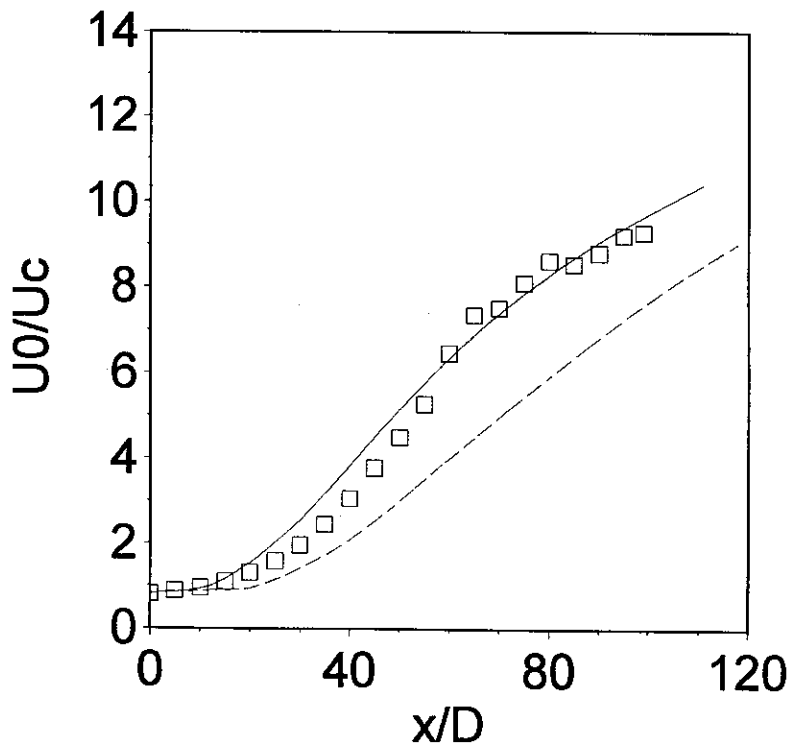
**Model B)** **pdf - mixing models ?**

# Effect of 'flowtype' correction on simulation on H3 diffusion flame

□ LDA : EKT
—— k-e standard
- - - - k-e with velocity divergence

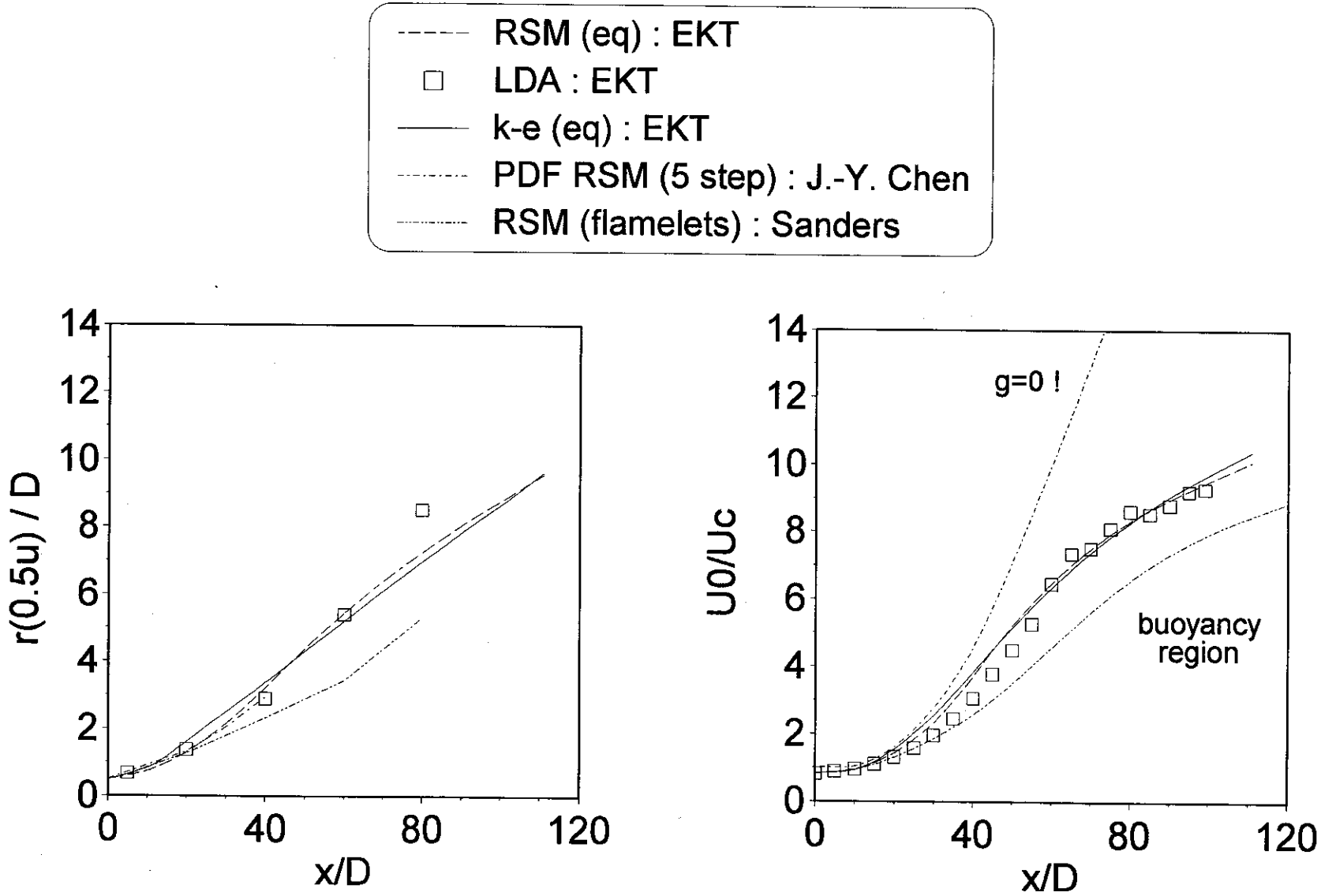
**=> Consequently, all corrections are only valid for one case!**



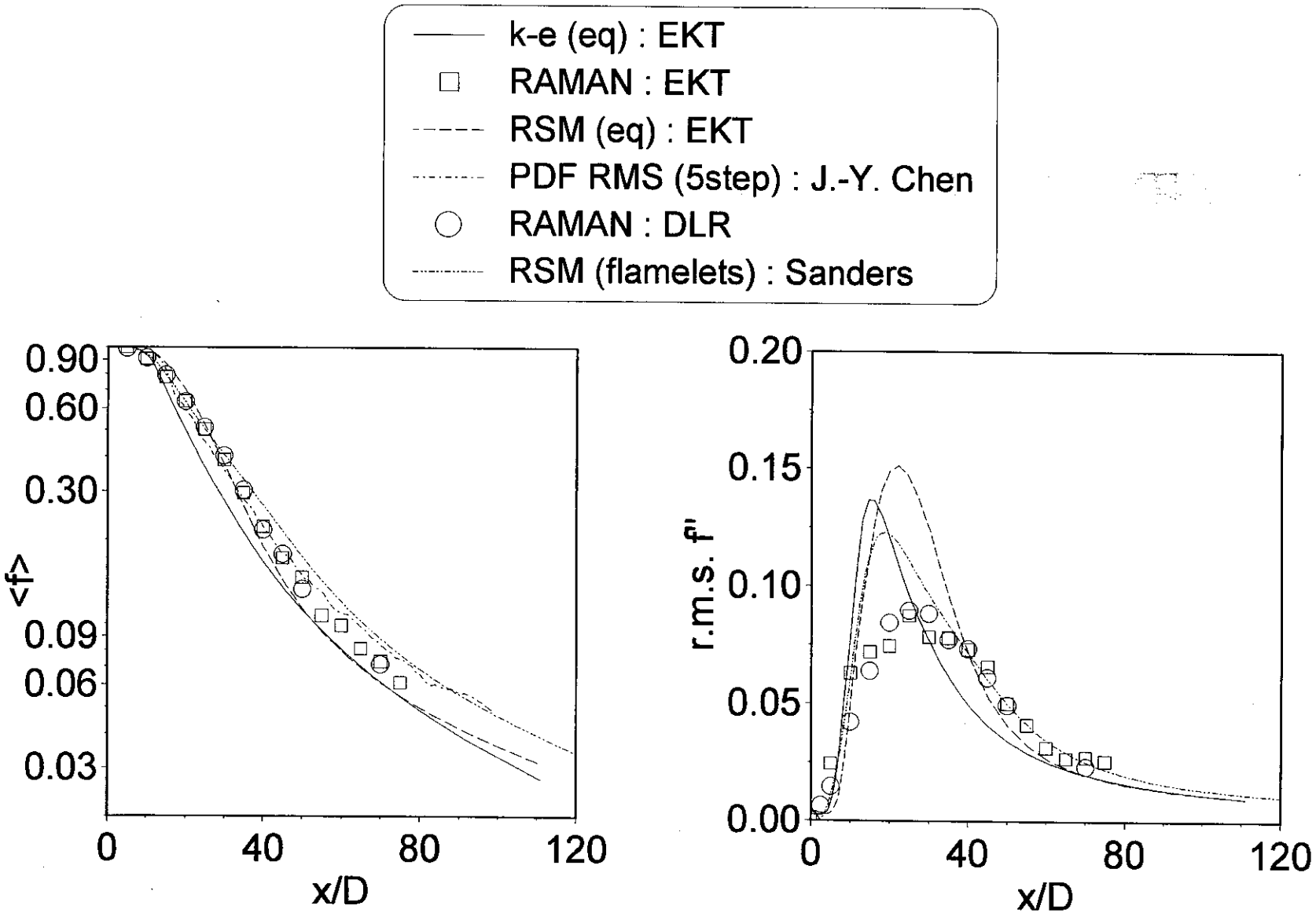
H3

# Spreading and centerline decay



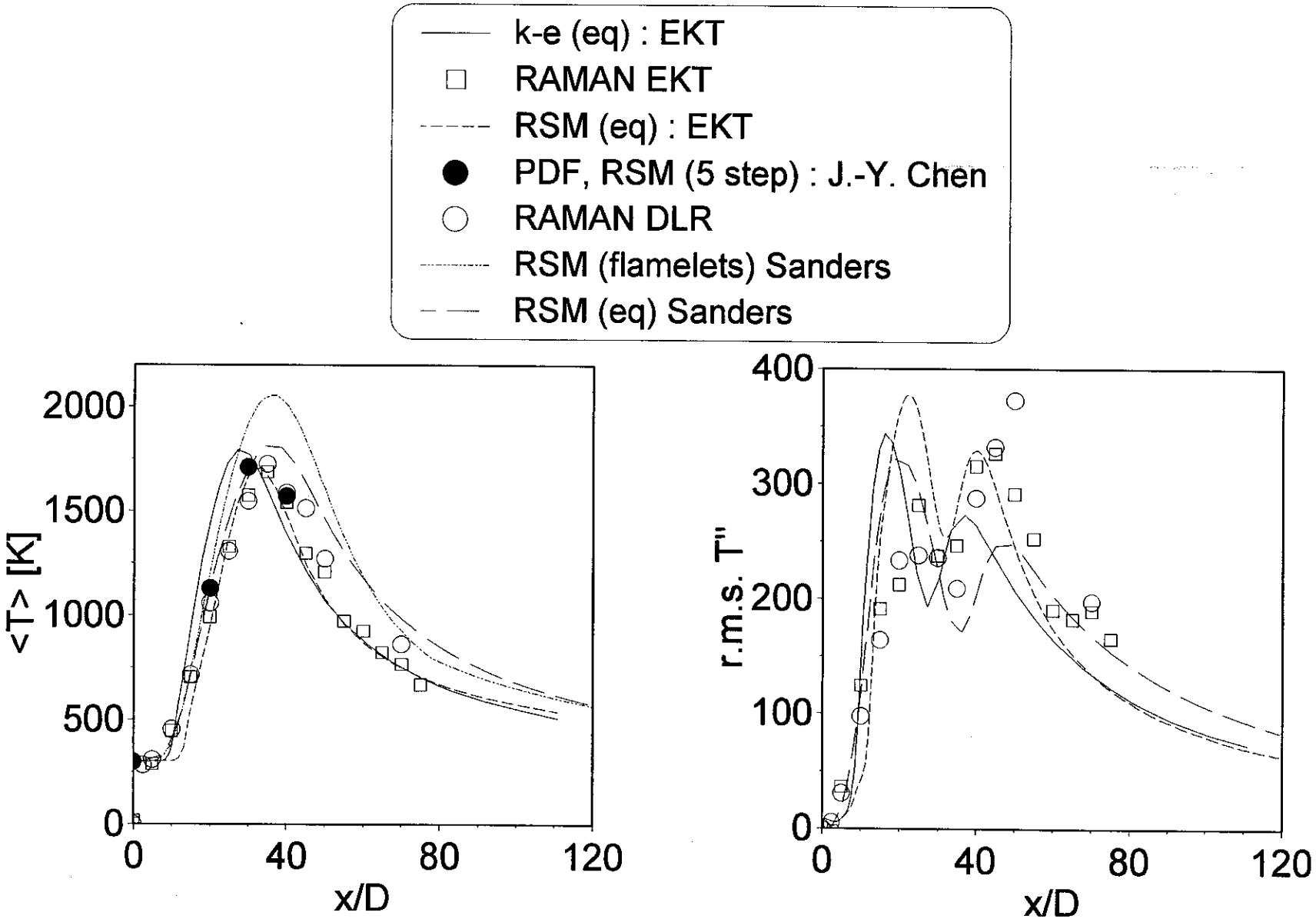
H3

# Favre averaged mixture fraction and r.m.s. along the axis



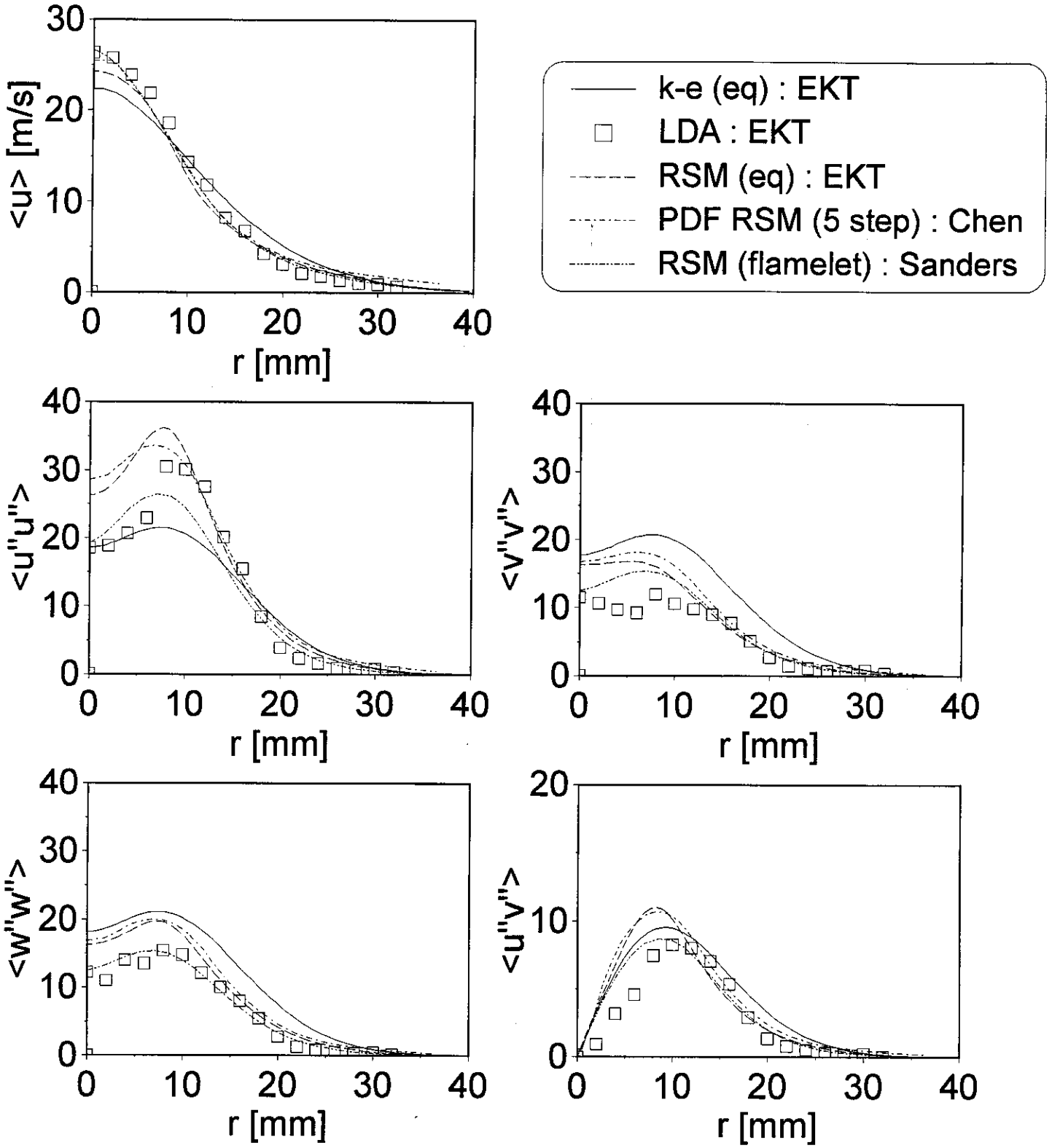
H3

# Favre averaged temperature and r.m.s. along the axis



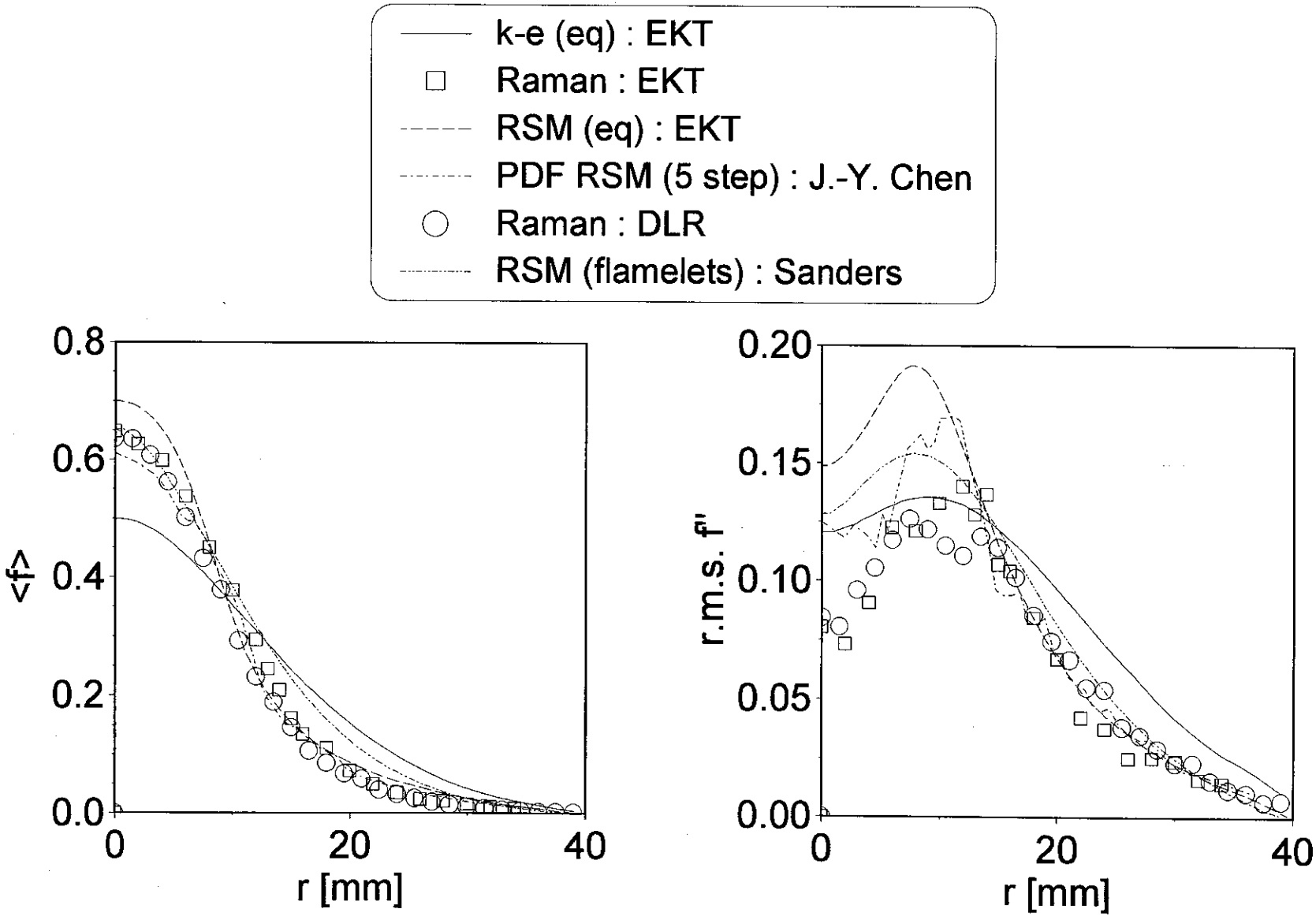
H3

# Favre averaged velocity and Reynolds stress tensor at x/D=20



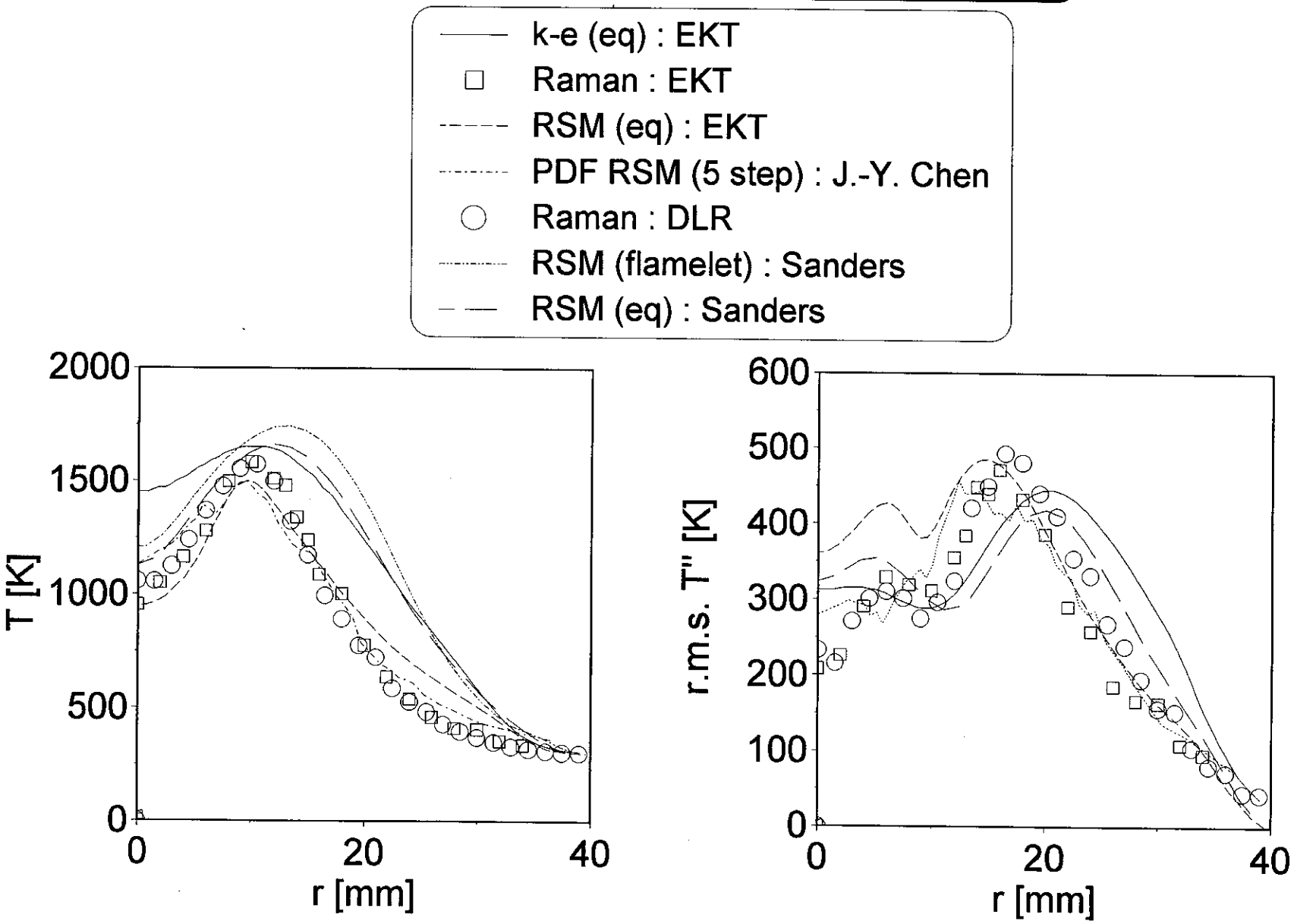
H3

# Favre averaged mixture fraction and r.m.s at X/D=20



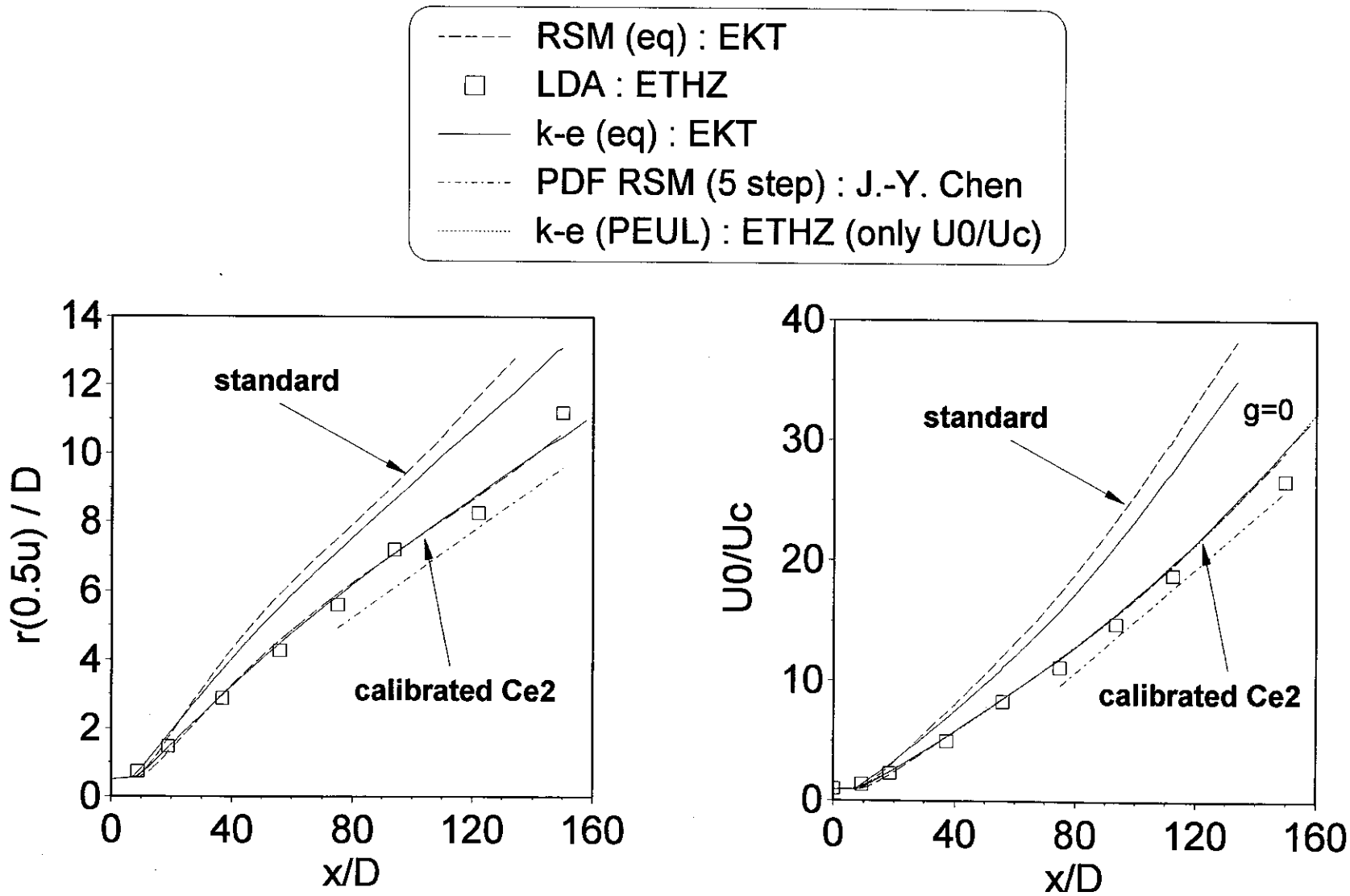
H3

# Favre averaged temperature and r.m.s. at x/D=20



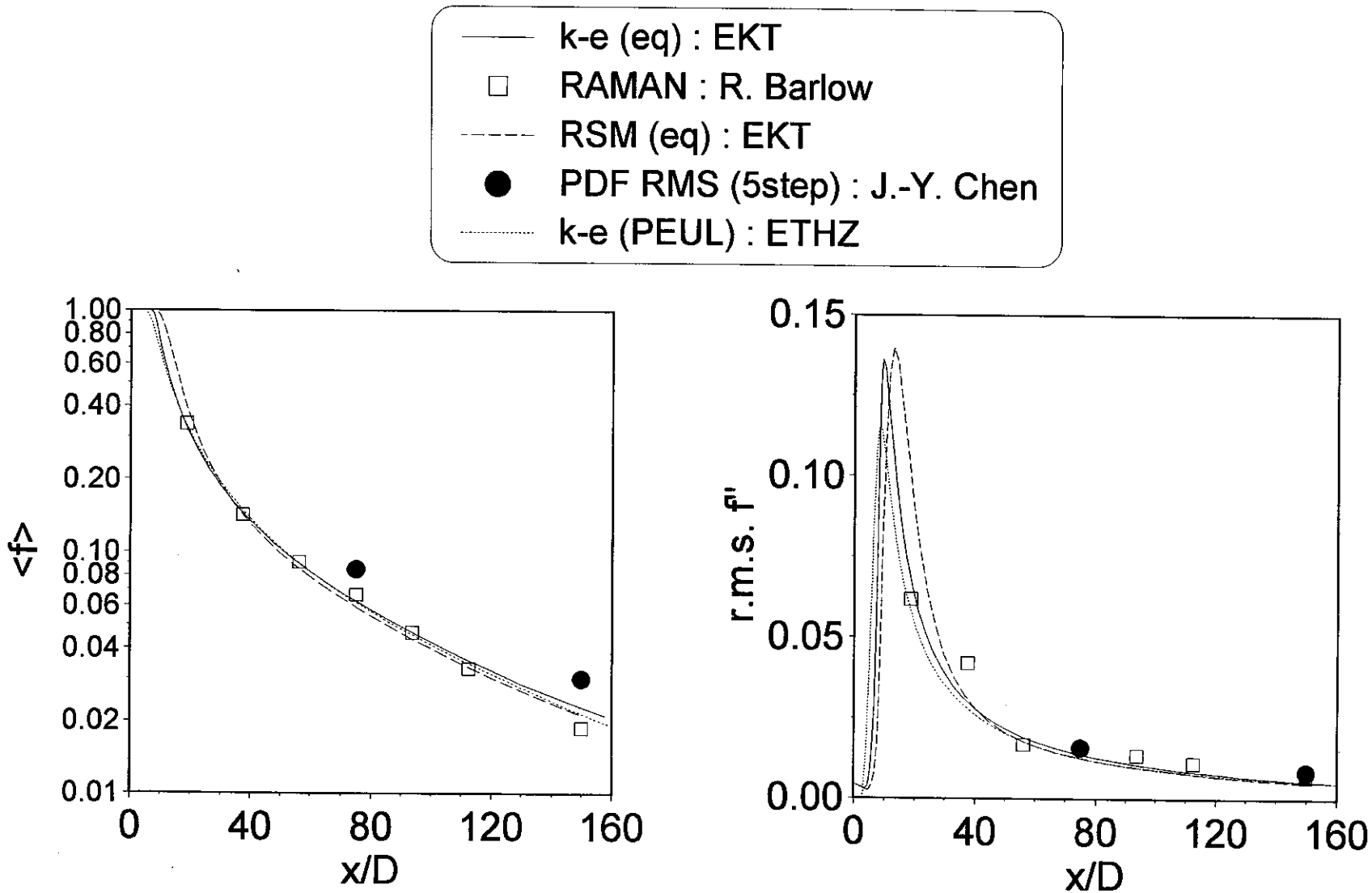
H2He20

# Spreading and centerline decay



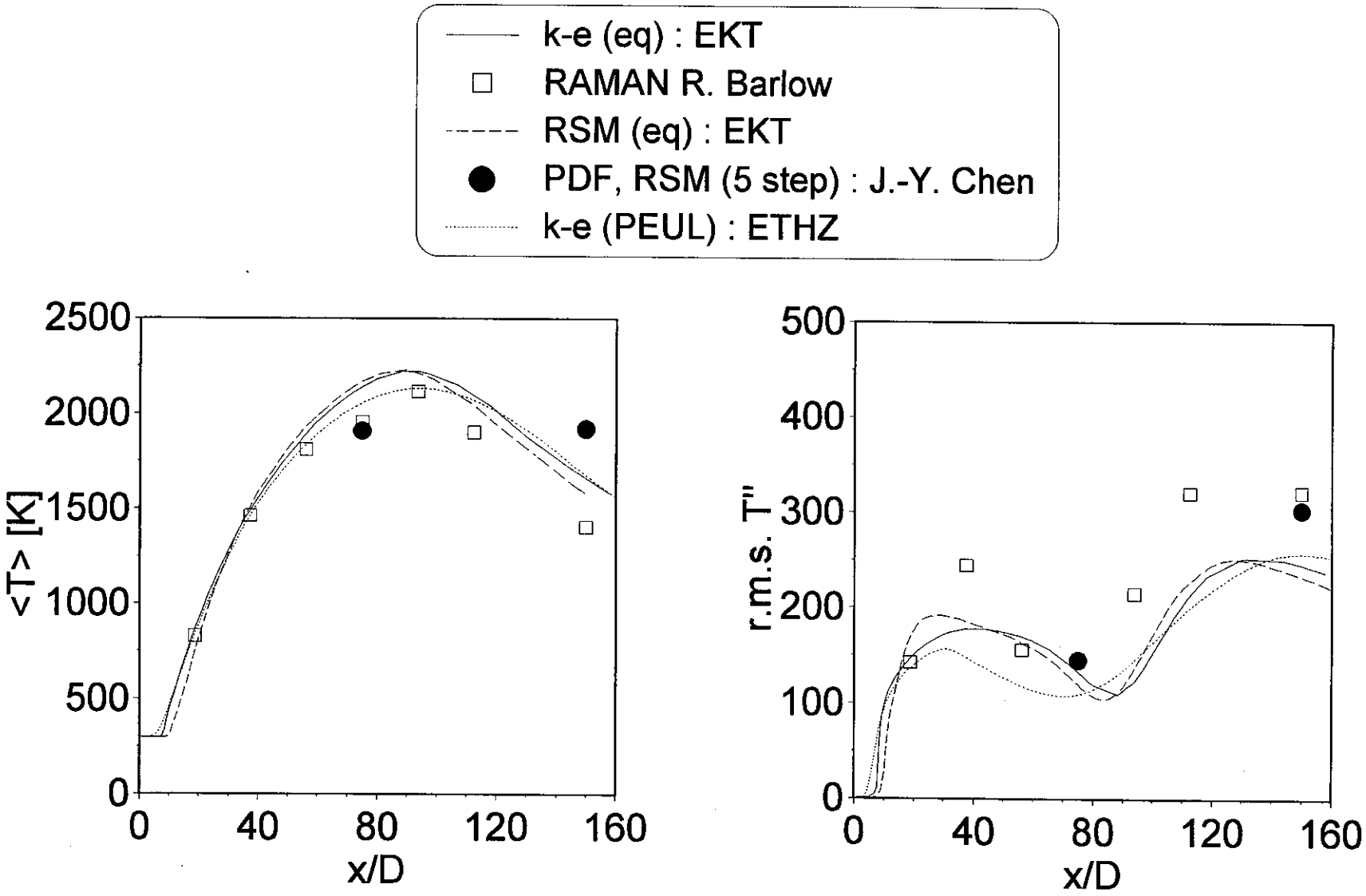
H2He20

# Favre averaged mixture fraction and r.m.s. along the axis



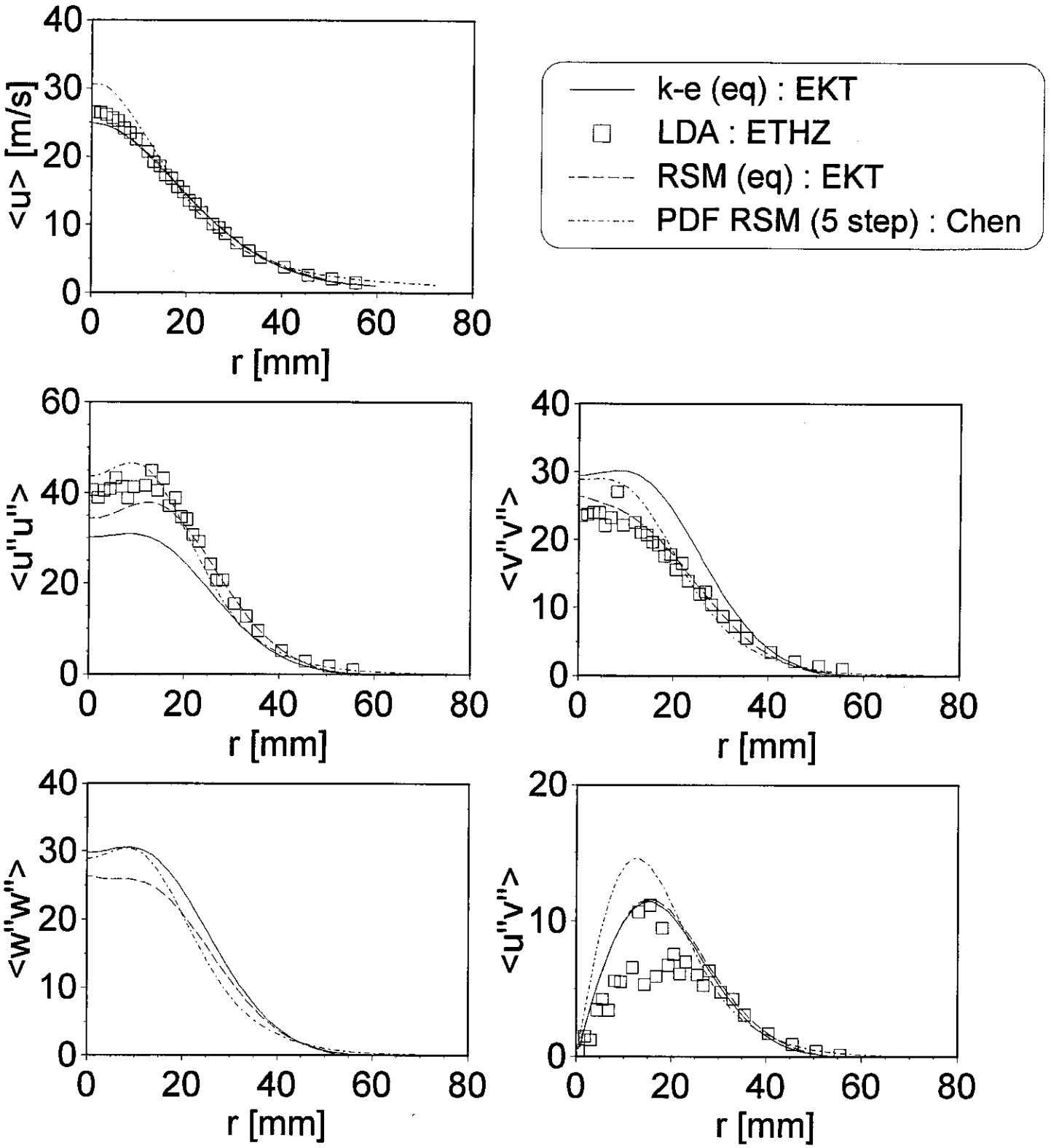
H2He20

# Favre averaged temperature and r.m.s. along the axis



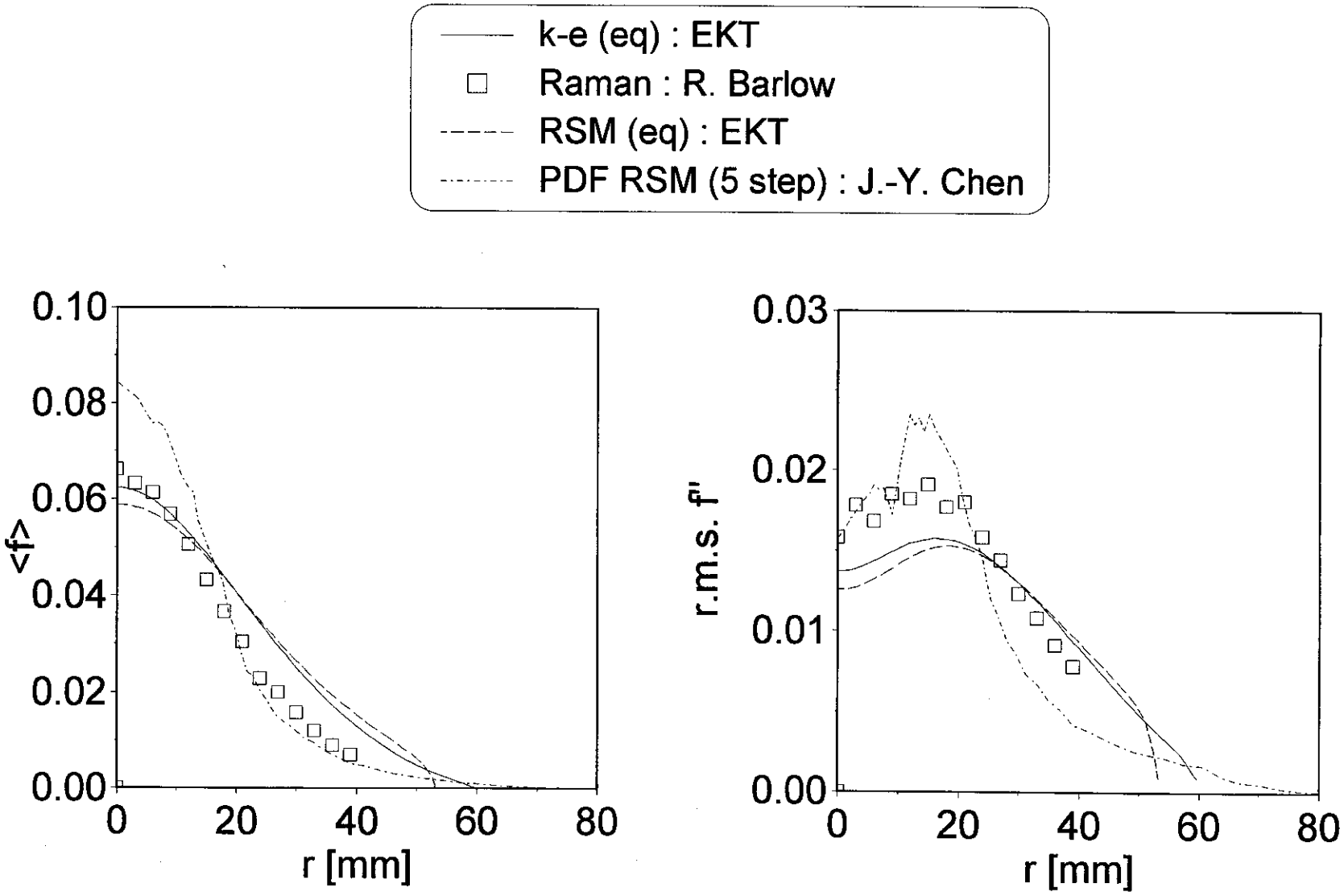
H2He20

# Favre averaged velocity and Reynolds stress tensor at x/D=75 = 1/2 L



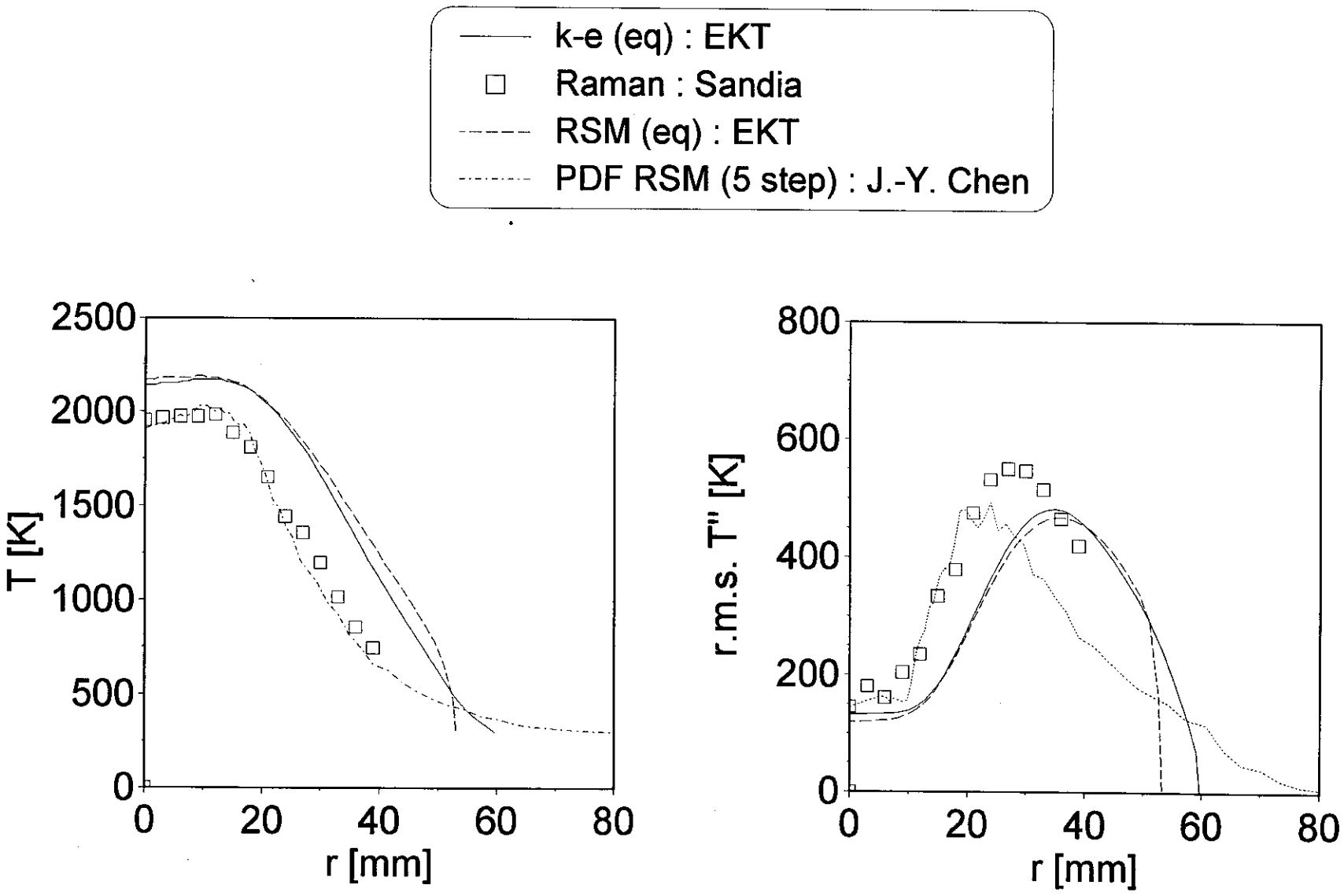
H2He20

# Favre averaged mixture fraction and r.m.s at x/D=75 = 1/2 L



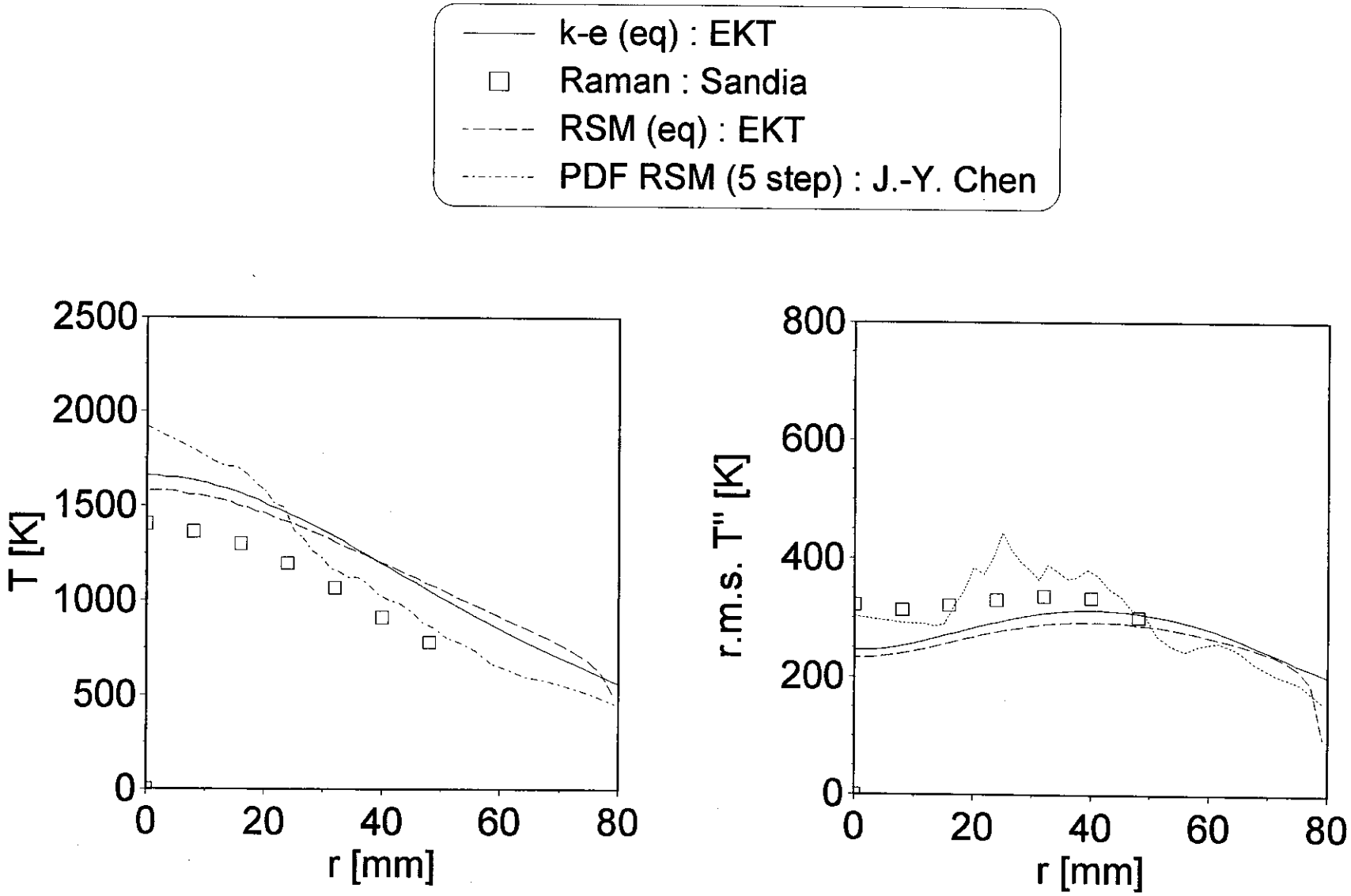
H2He20

# Favre averaged temperature and r.m.s. at x/D=75 = 1/2 L



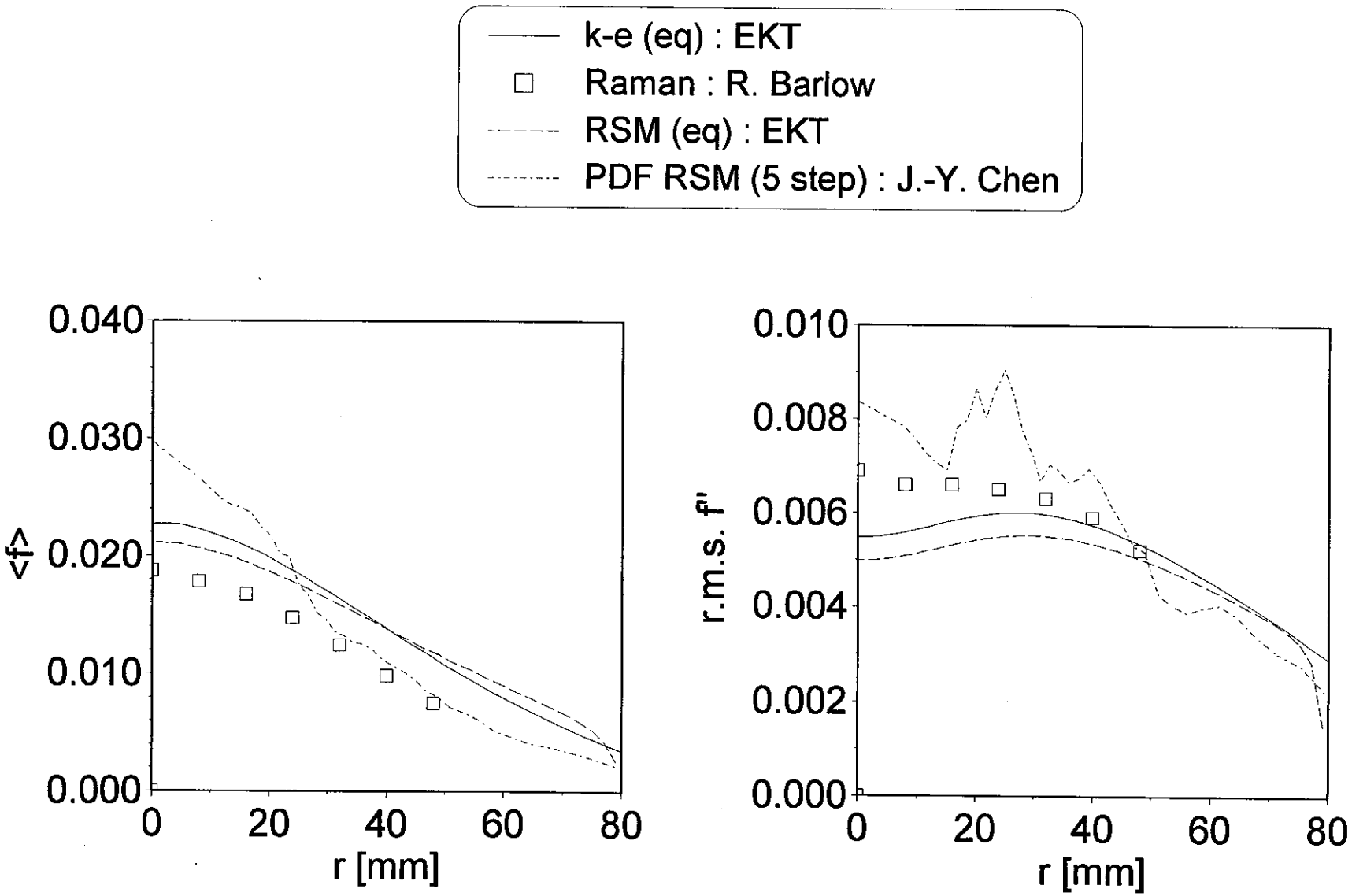
H2He20

# Favre averaged temperature and r.m.s. at x/D=150 = 1/1 L



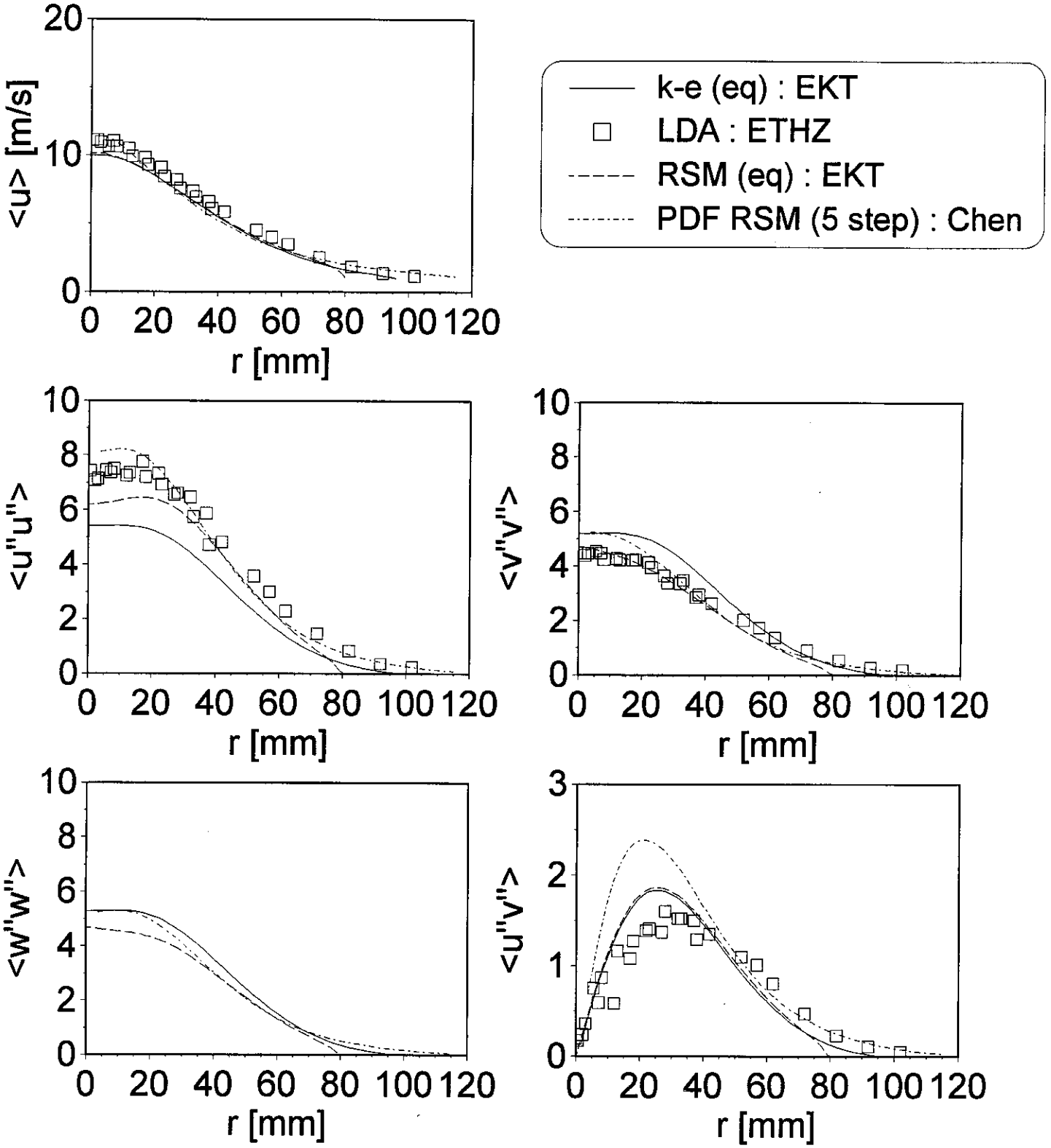
H2He20

# Favre averaged mixture fraction and r.m.s at x/D=150 = 1/1 L



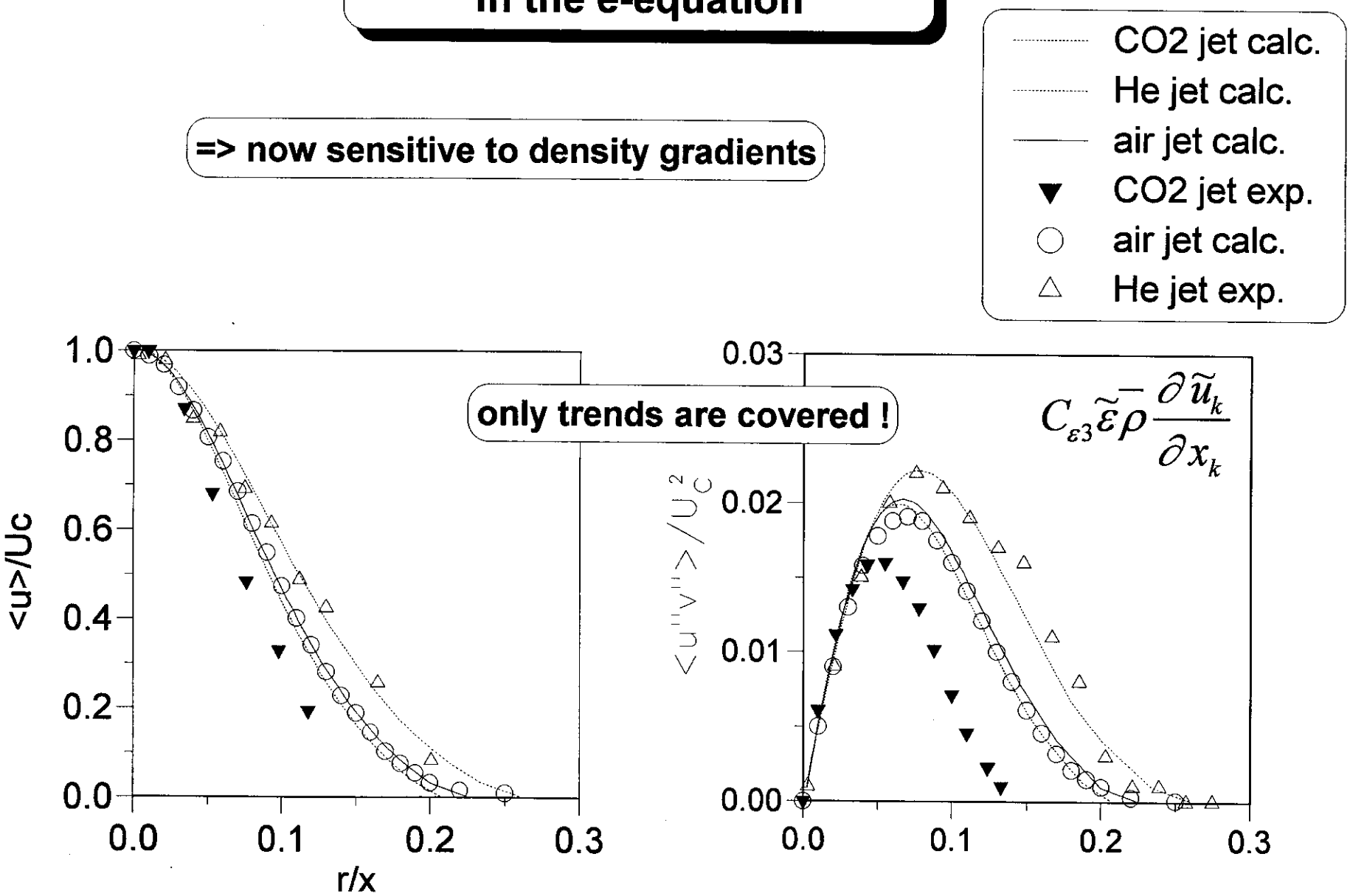
**H2He20**

# Favre averaged velocity and Reynolds stress tensor at x/D=150 = 1/1 L



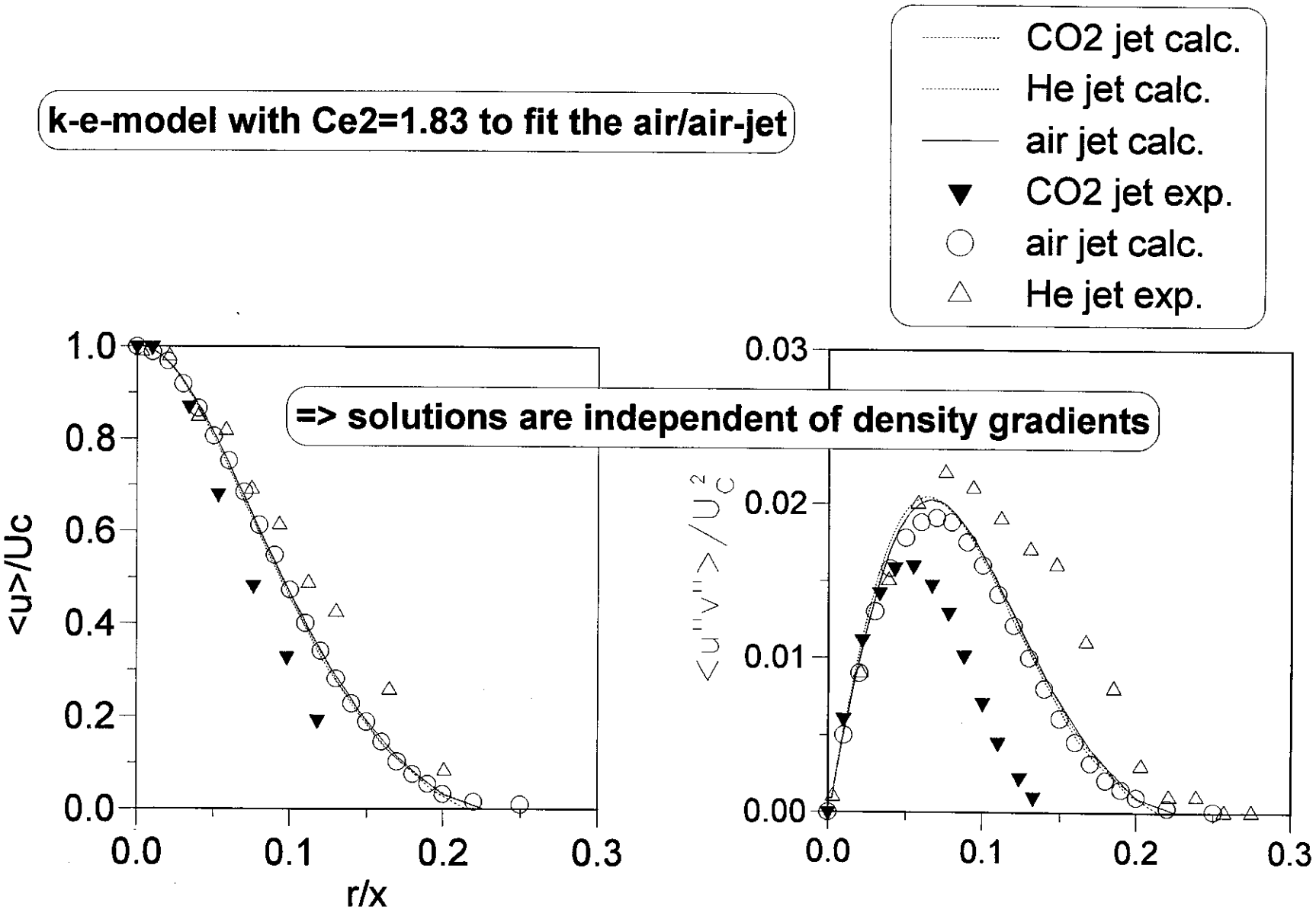
# The k-e model extended by a velocity divergence term in the e-equation

=> now sensitive to density gradients



# The standard k-e-model and variable density round jets

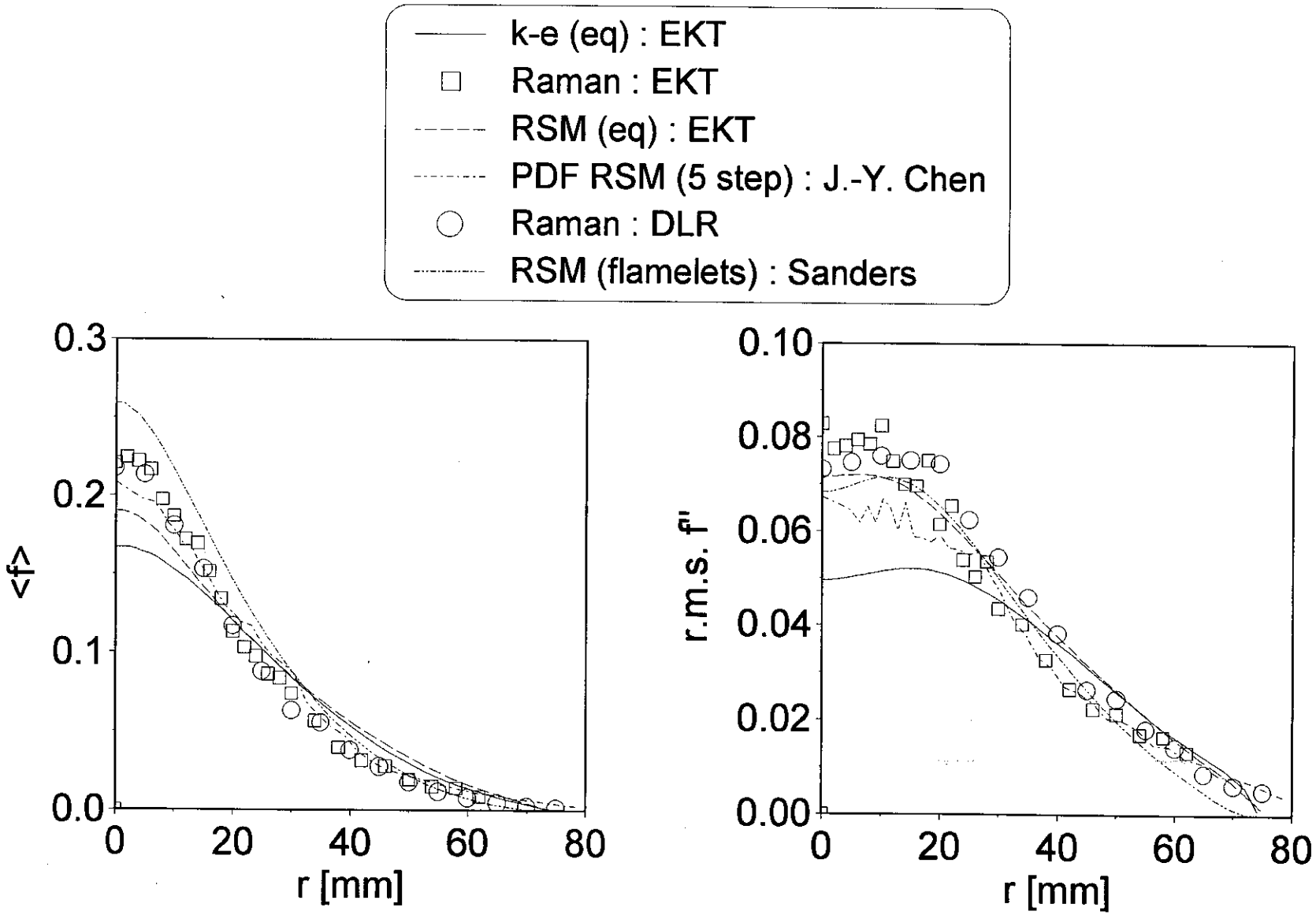
**k-e-model with Ce2=1.83 to fit the air/air-jet**




**=> solutions are independent of density gradients**

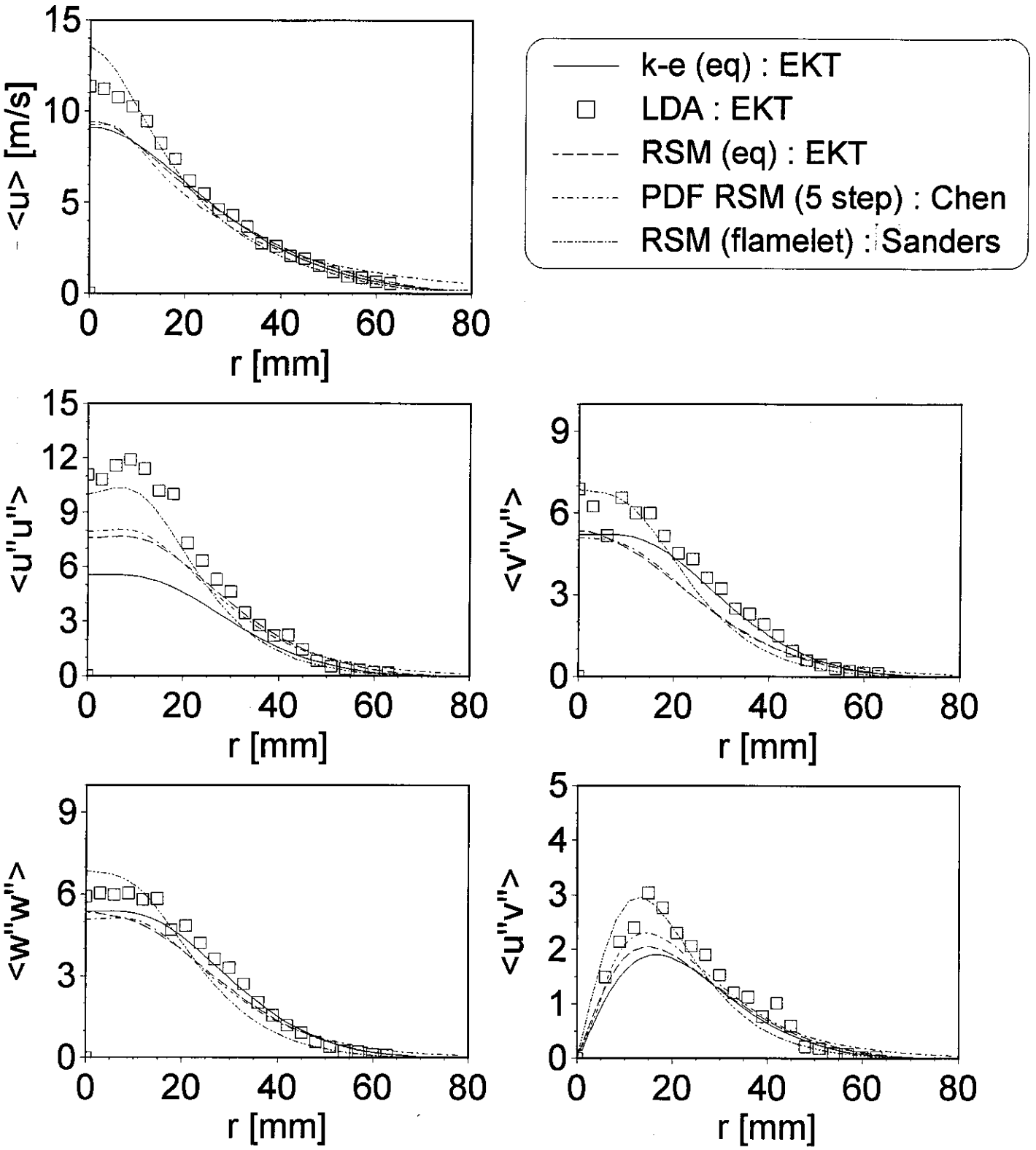
H3

# Favre averaged mixture fraction and r.m.s at X/D=40



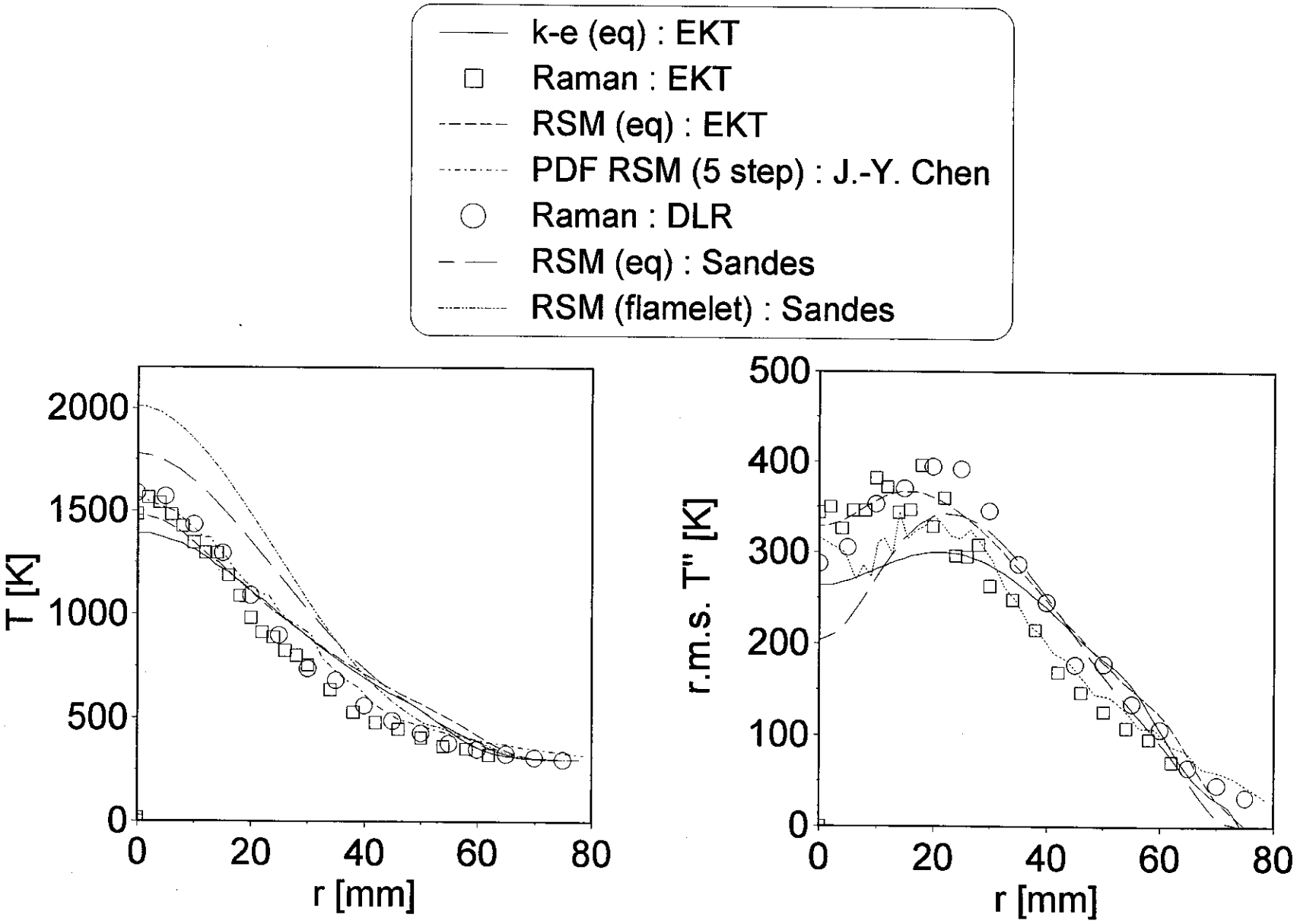
H3

# Favre averaged velocity and Reynolds stress tensor at x/D=40

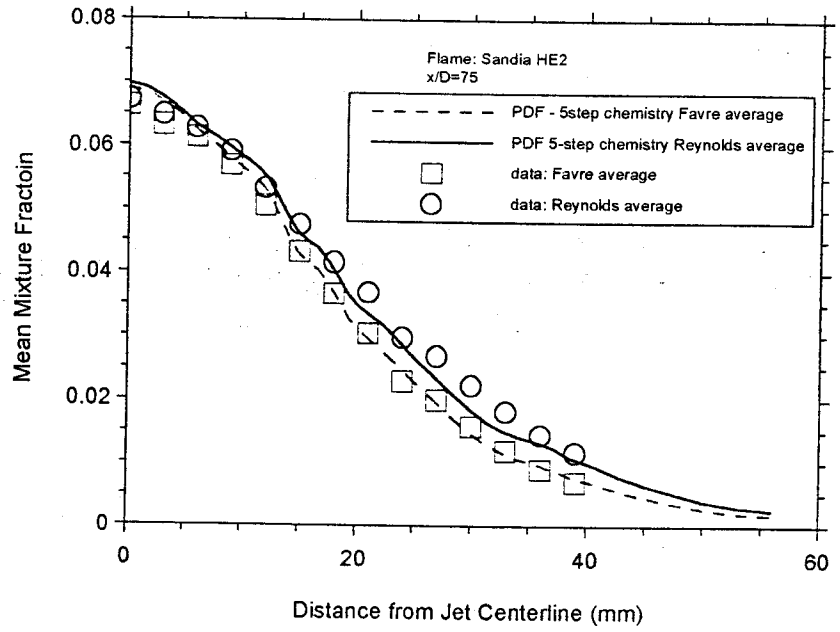


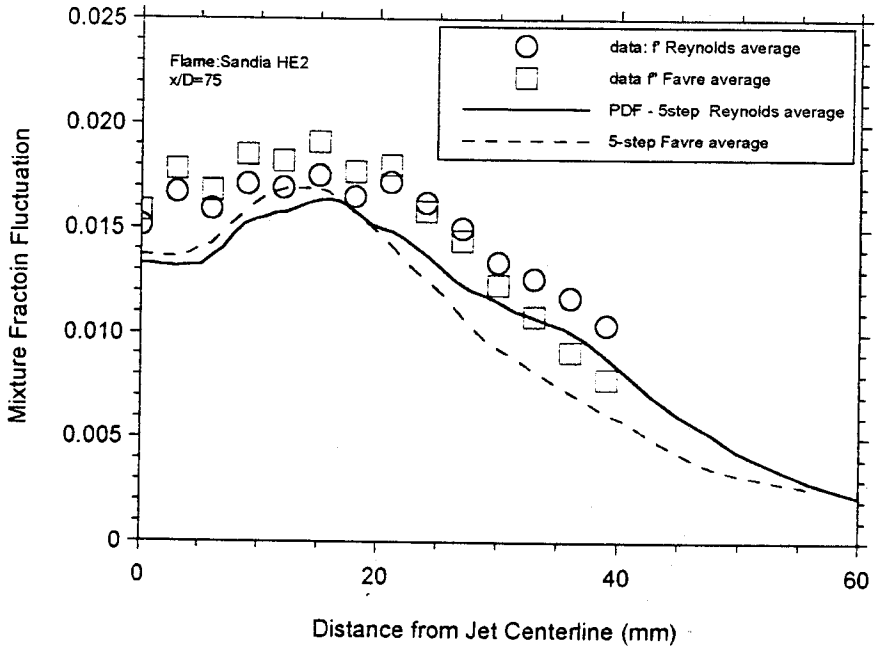
H3

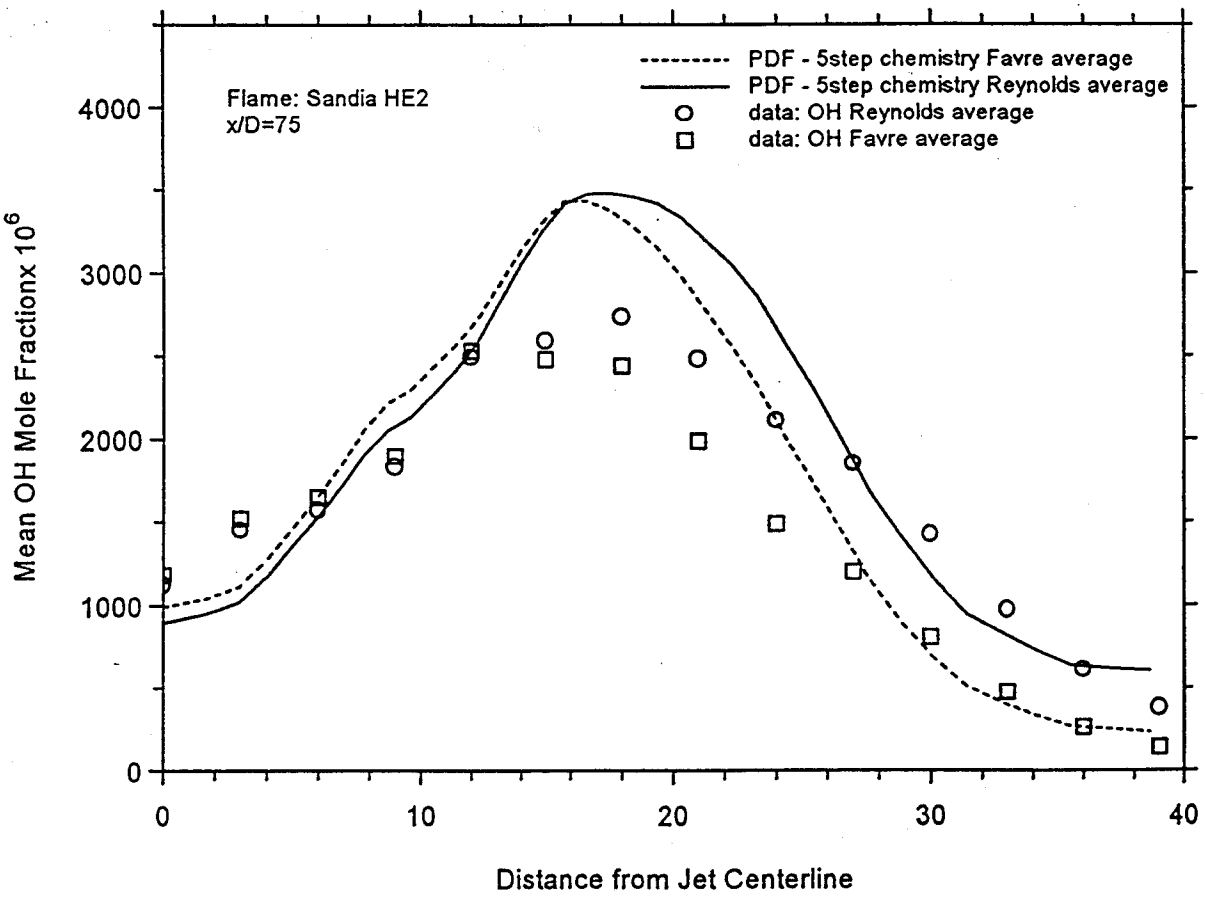
# Favre averaged temperature and r.m.s. at x/D=40

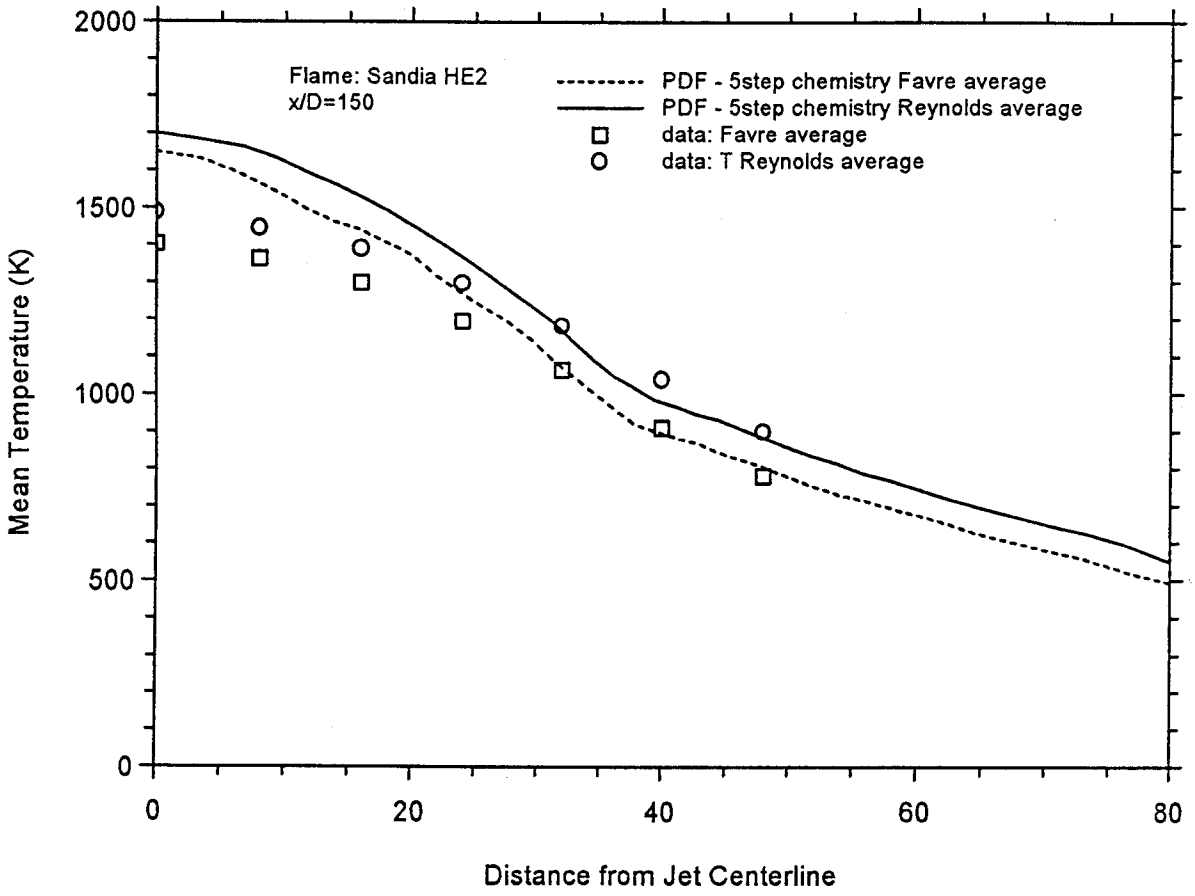


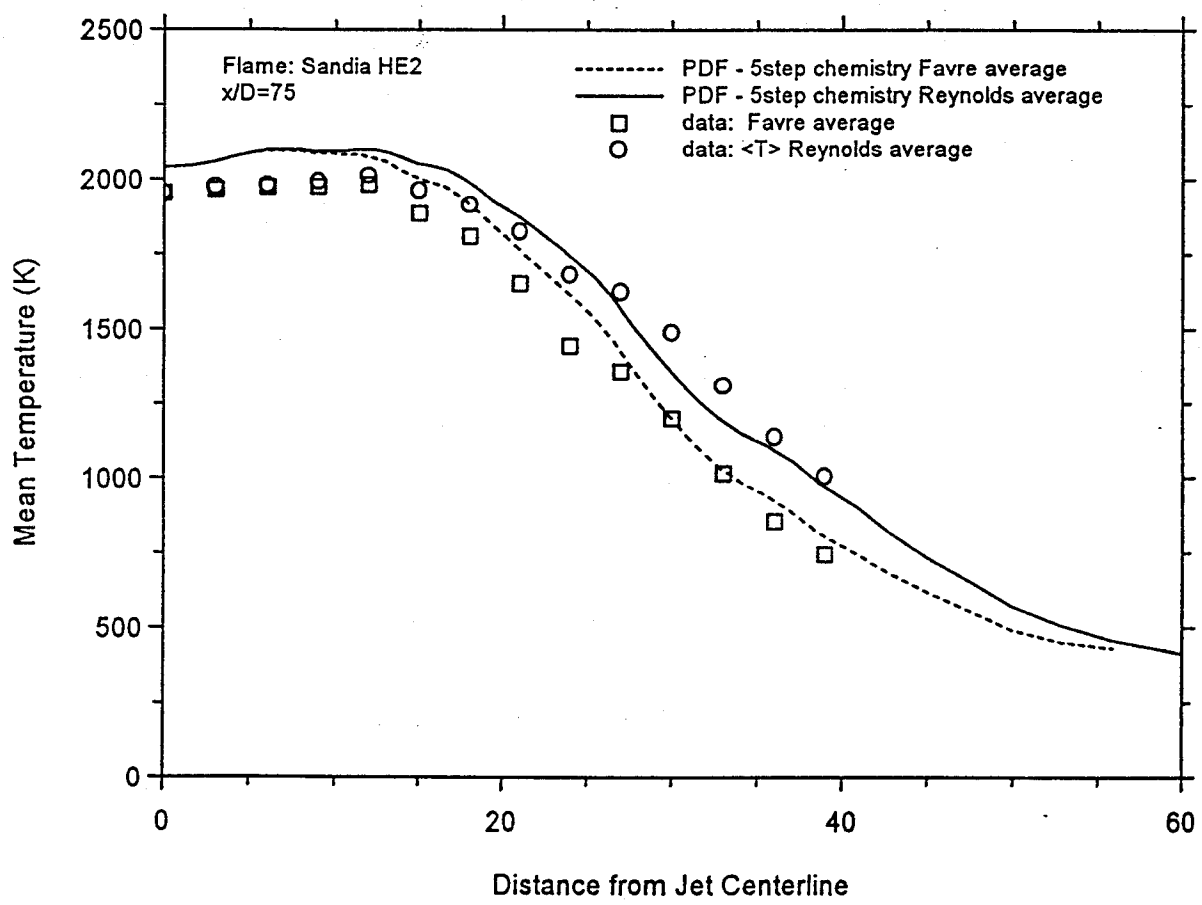
# Sandia 20%Helium+80%$H_2$ Turbulent Jet Flame
## x/D=75 (1/2 Visible Flame Height )

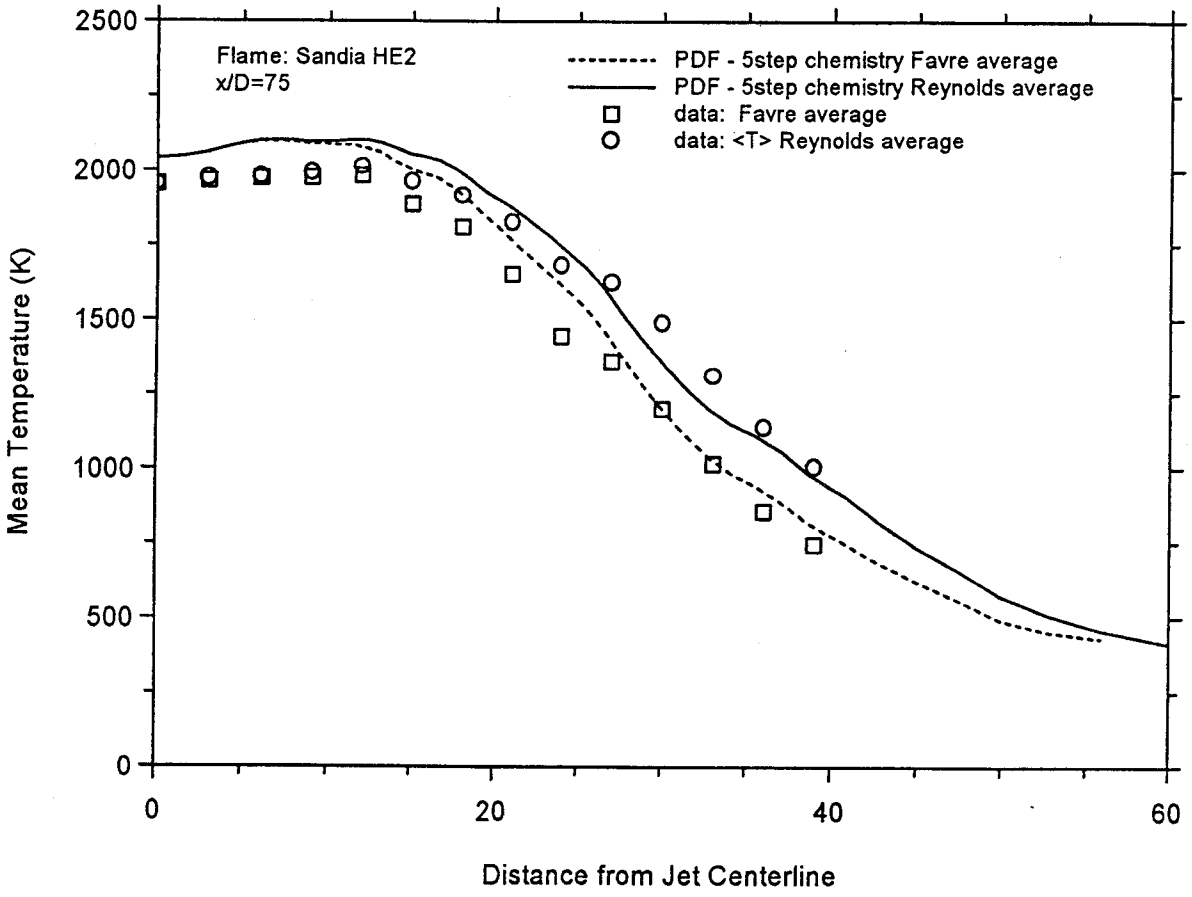


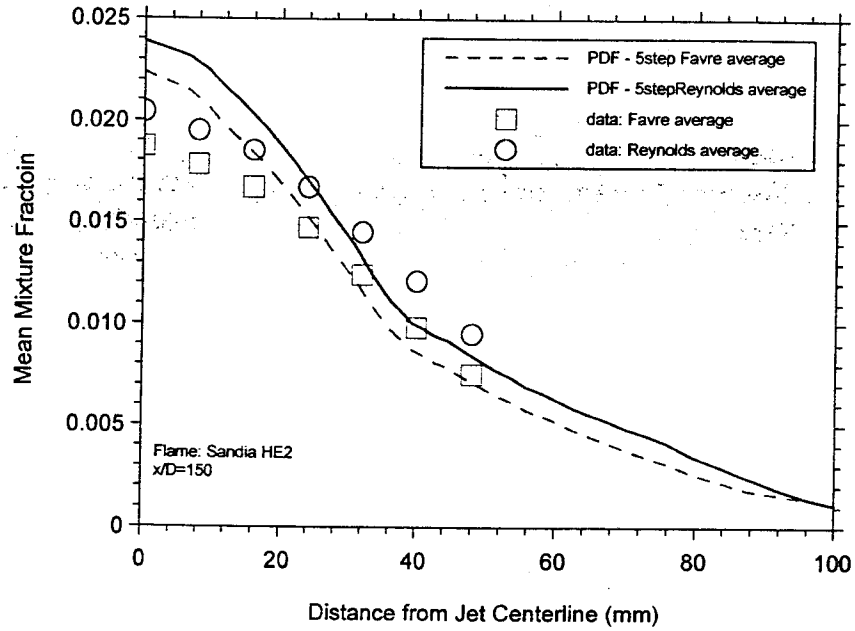

PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: OH Reynolds average
data: OH Favre average
Flame: Sandia HE2
x/D=75
Mean OH Mole Fractionx 10^6
4000
3000
2000
1000
0
0
10
20
30
40
Distance from Jet Centerline

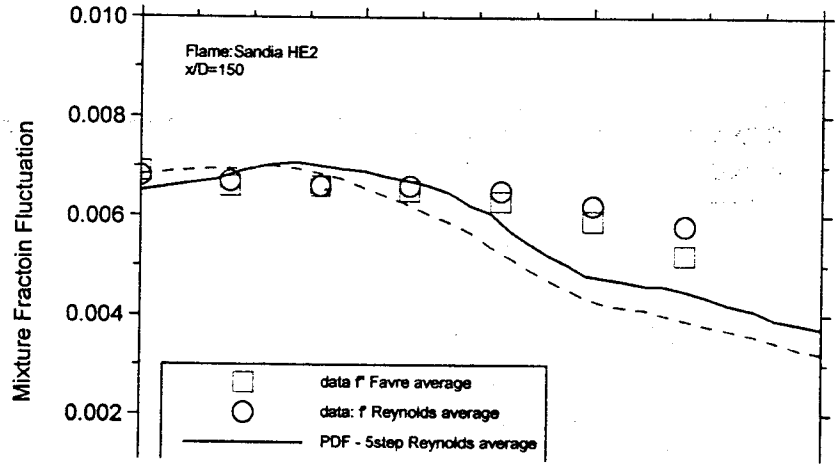

Flame: Sandia HE2
x/D=150
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: Favre average
data: T Reynolds average
Mean Temperature (K)
2000
1500
1000
500
0
0
20
40
60
80
Distance from Jet Centerline

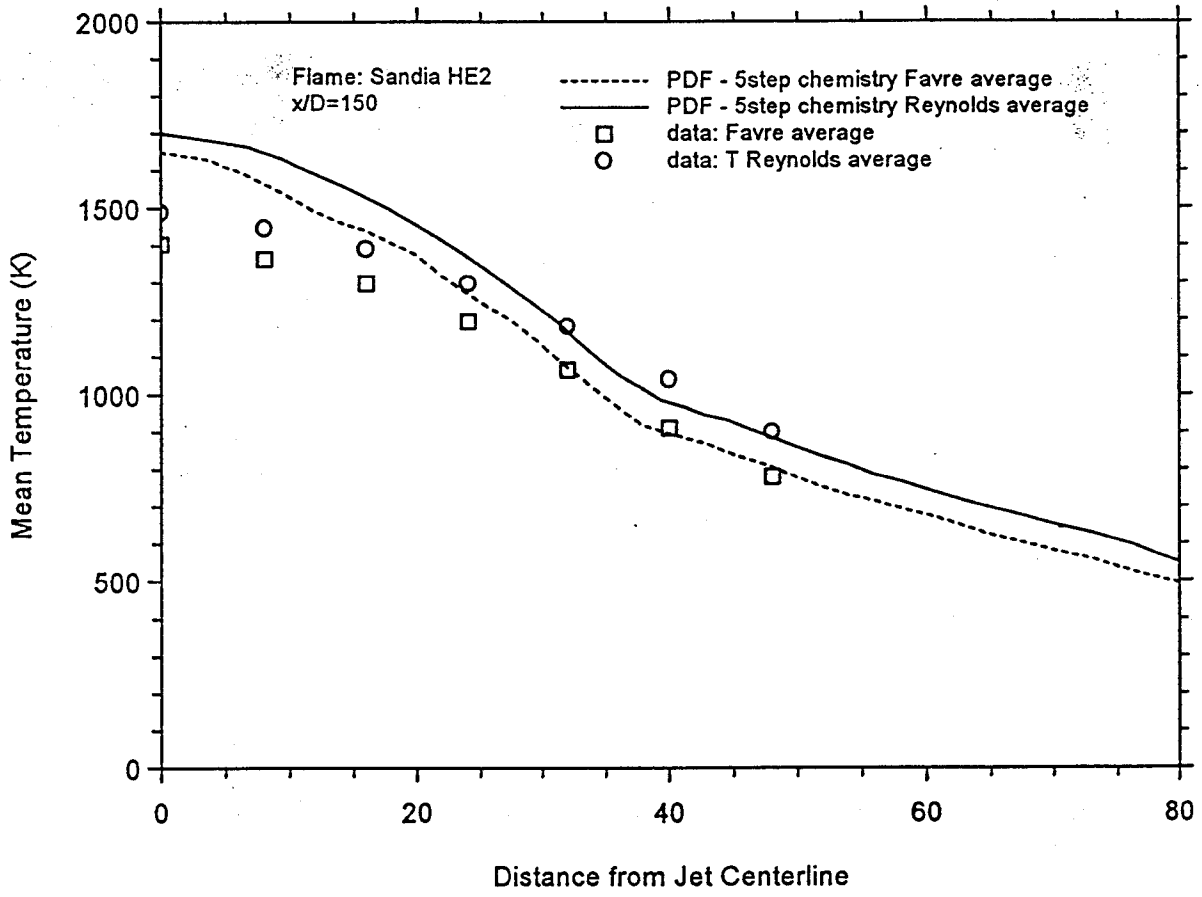

Flame: Sandia HE2
x/D=75
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: Favre average
data: <T> Reynolds average
Mean Temperature (K)
2500
2000
1500
1000
500
0
0
20
40
60
Distance from Jet Centerline


Flame: Sandia HE2
x/D=75
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: Favre average
data: <T> Reynolds average
Mean Temperature (K)
2500
2000
1500
1000
500
0
0
20
40
60
Distance from Jet Centerline

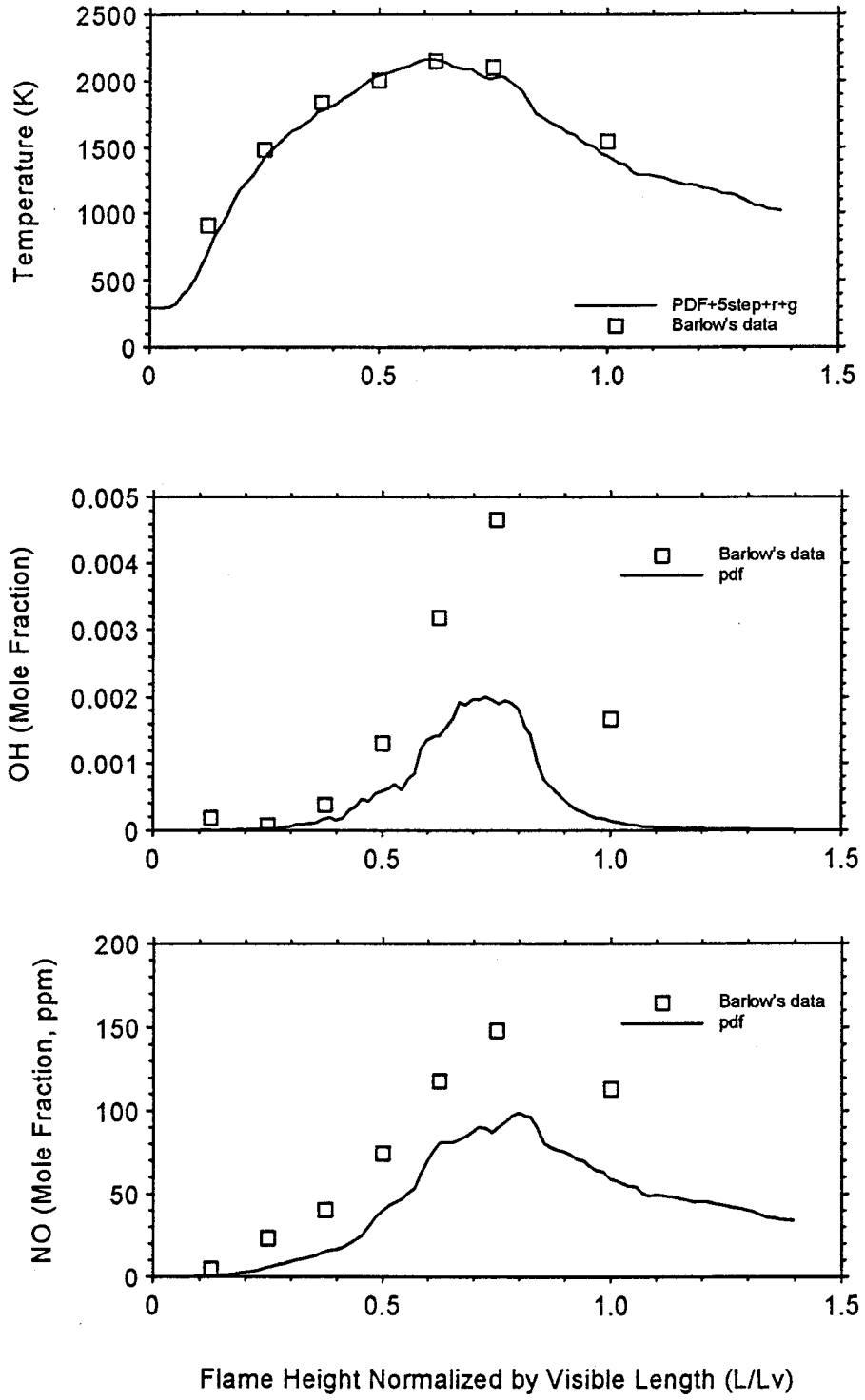
# Sandia 20%Helium+80%$H_2$ Turbulent Jet Flame
## x/D=150 (Visible Flame Height)

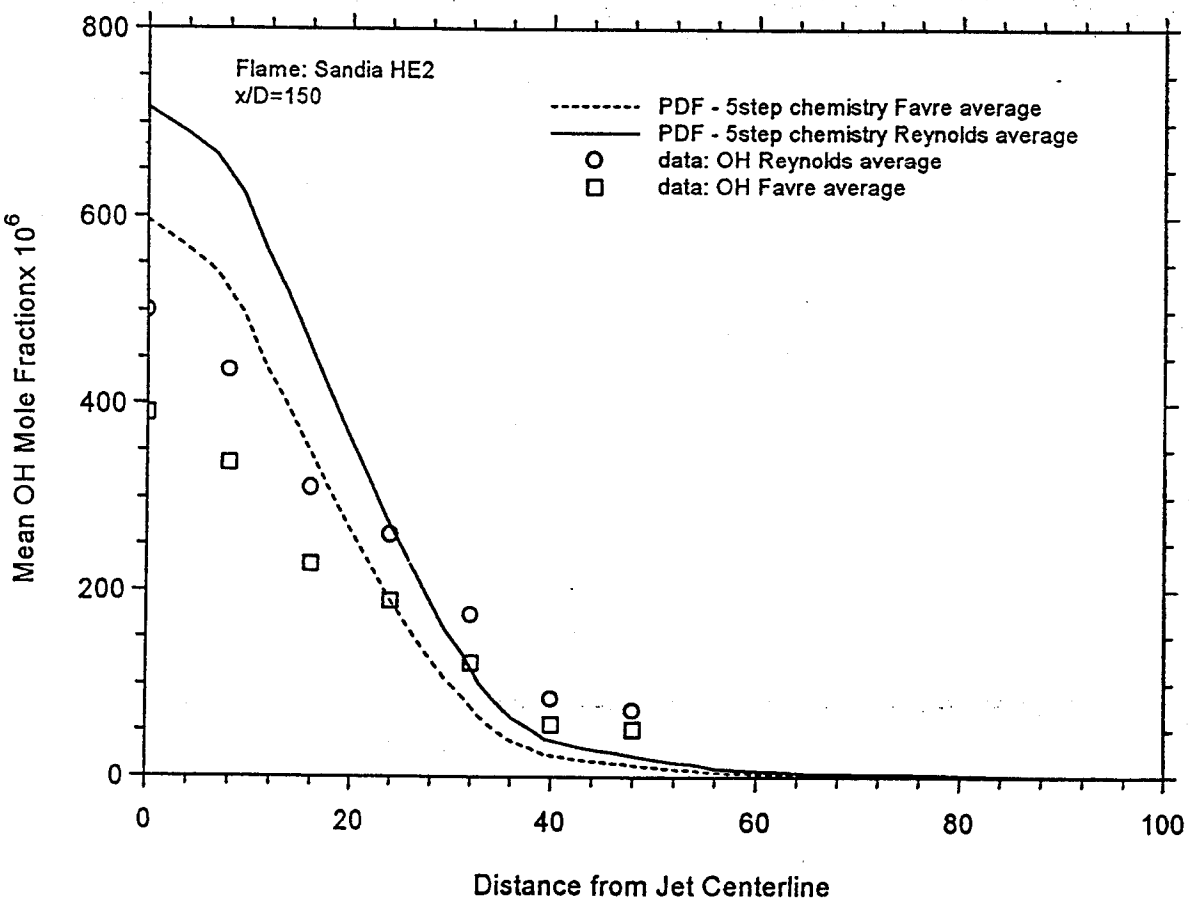


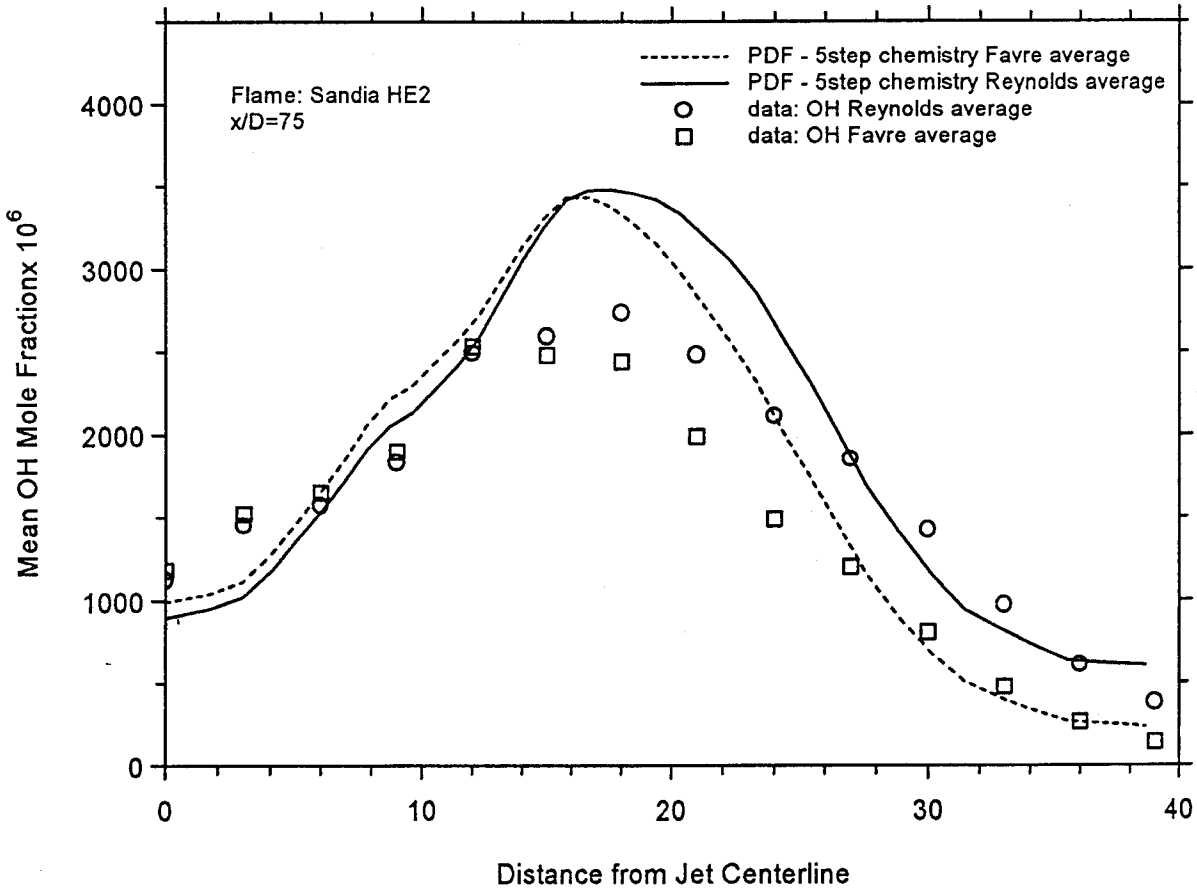




Flame: Sandia HE2
x/D=150
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: Favre average
data: T Reynolds average
Mean Temperature (K)
2000
1500
1000
500
0
0
20
40
60
80
Distance from Jet Centerline

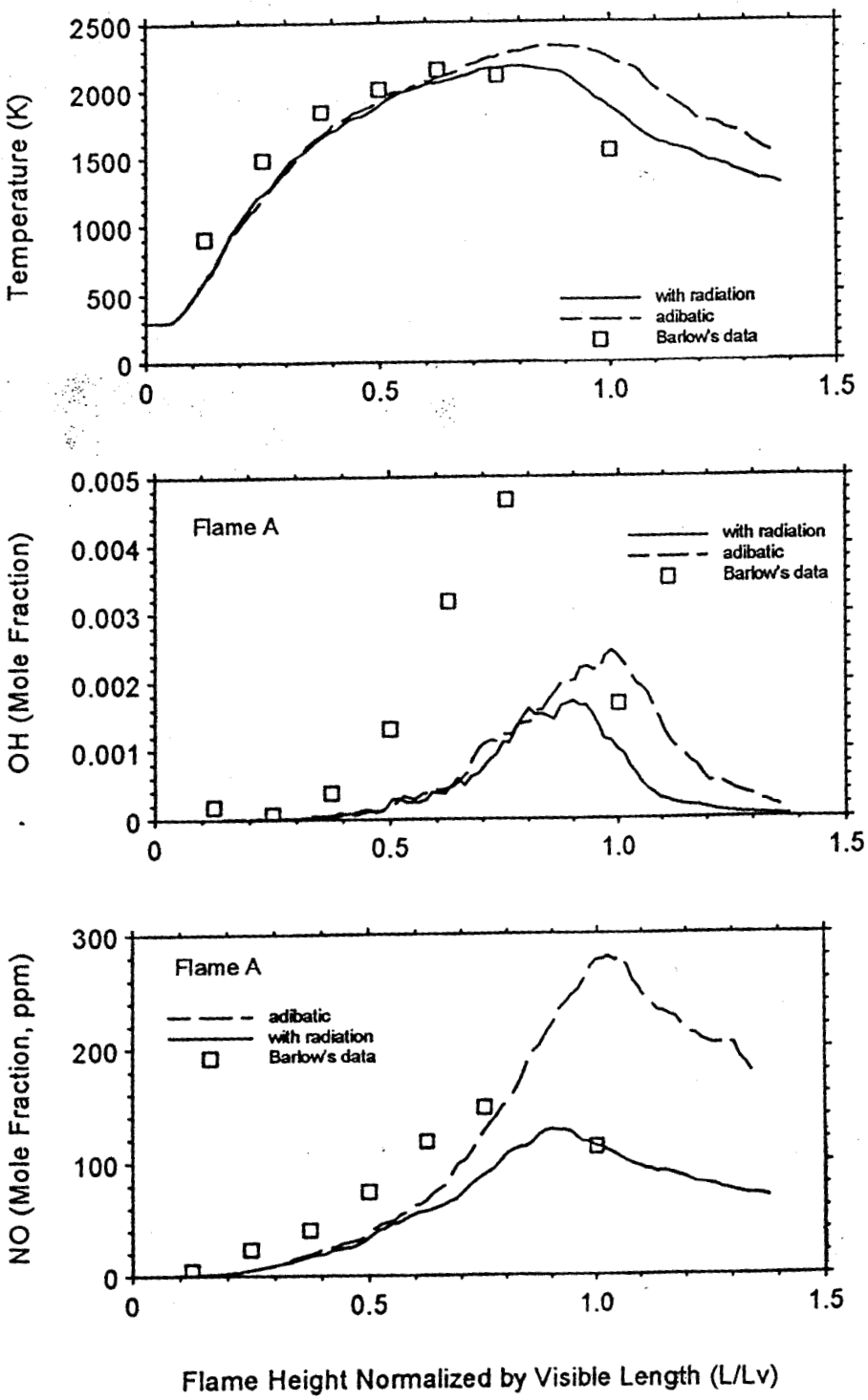
# Pure H2 Jet flame: PDF +5step CCOr=0.02+r+g

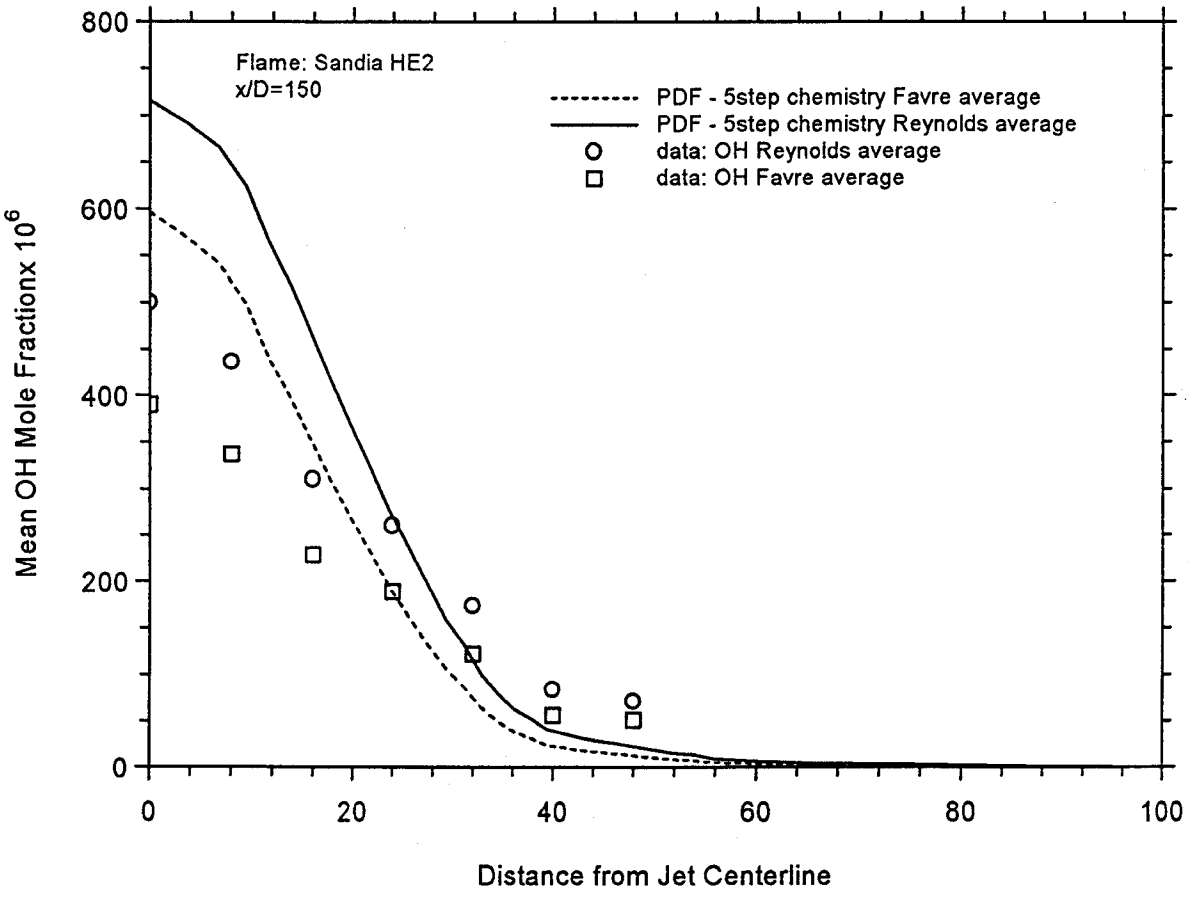



Flame: Sandia HE2
x/D=150
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: OH Reynolds average
data: OH Favre average
Mean OH Mole Fractionx 10^6
Distance from Jet Centerline
0
200
400
600
800
0
20
40
60
80
100

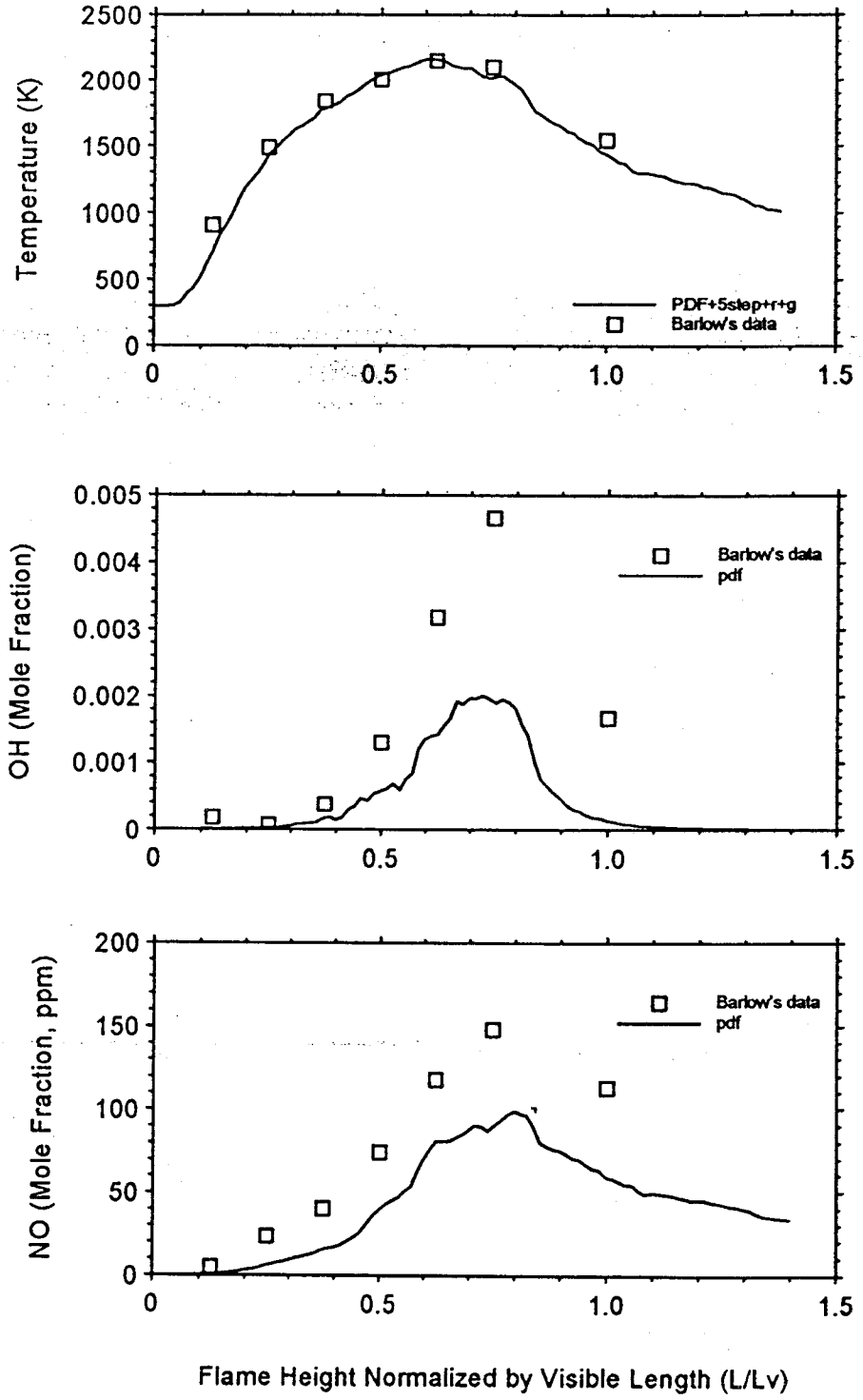

PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: OH Reynolds average
data: OH Favre average
Flame: Sandia HE2
x/D=75
Mean OH Mole Fractionx 10^6
4000
3000
2000
1000
0
0
10
20
30
40
Distance from Jet Centerline

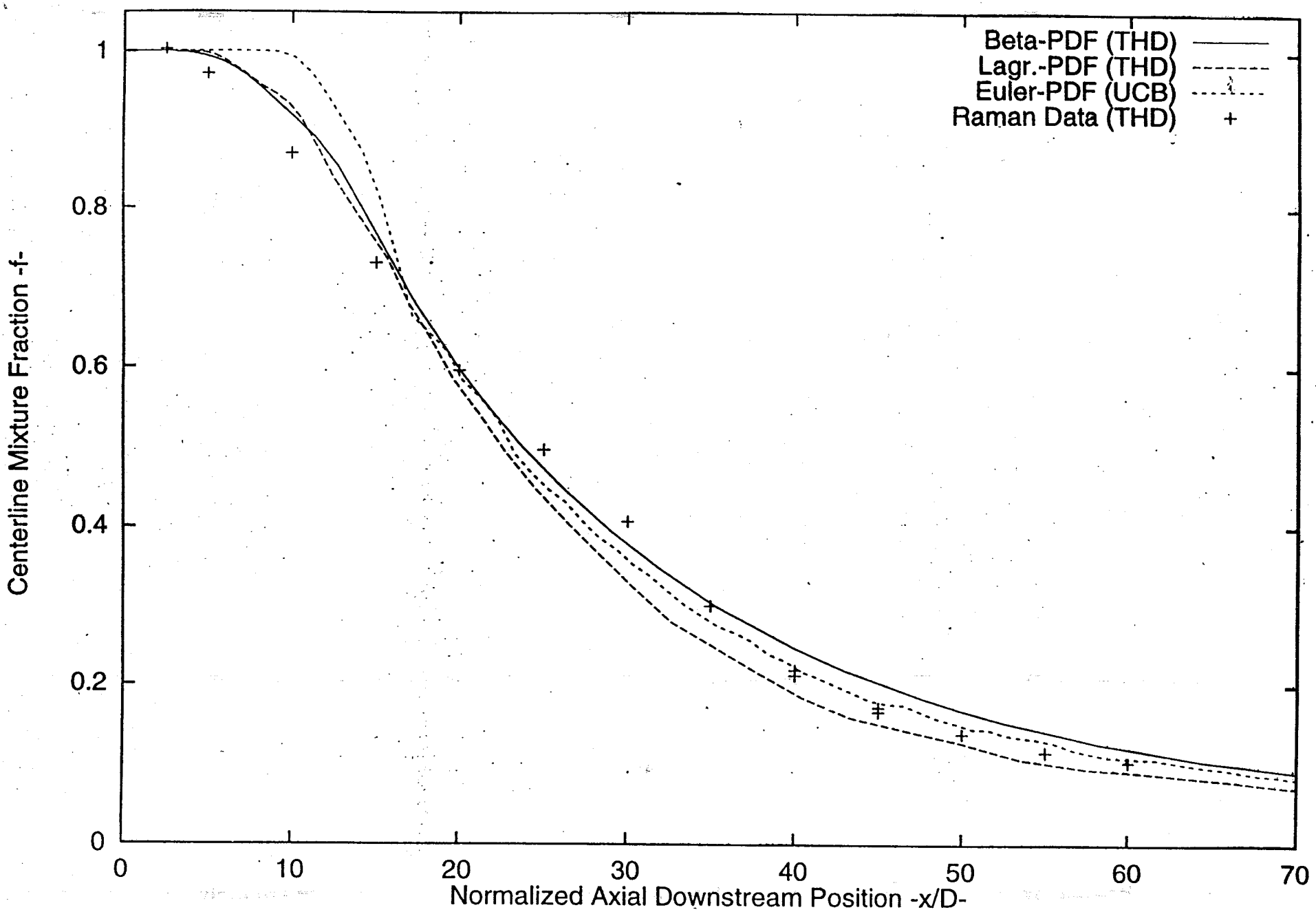
# Pure H2 Jet flame: PDF +5step CCOr=0.04

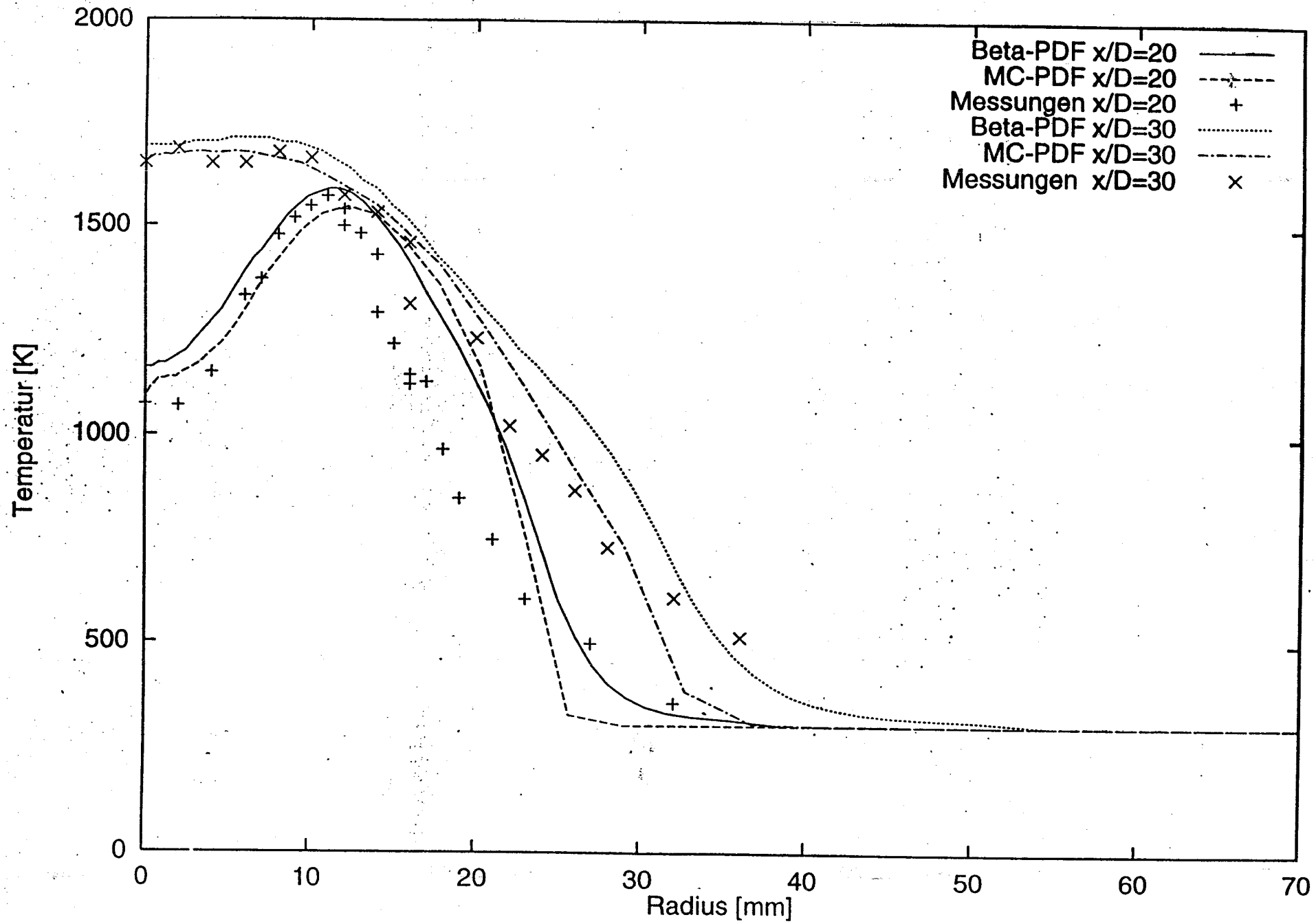


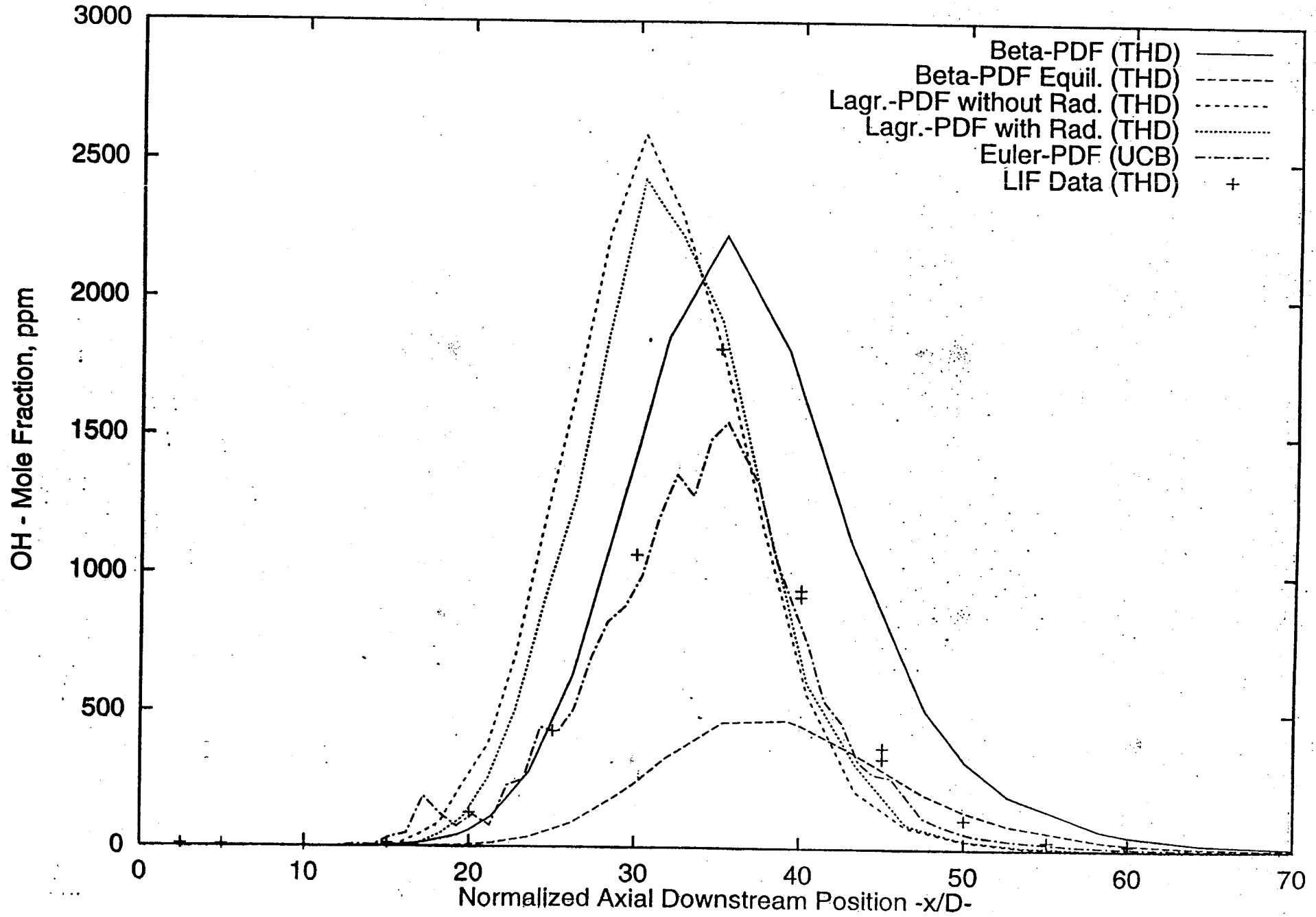

Flame: Sandia HE2
x/D=150
PDF - 5step chemistry Favre average
PDF - 5step chemistry Reynolds average
data: OH Reynolds average
data: OH Favre average
Mean OH Mole Fractionx 10^6
Distance from Jet Centerline
0
200
400
600
800
0
20
40
60
80
100

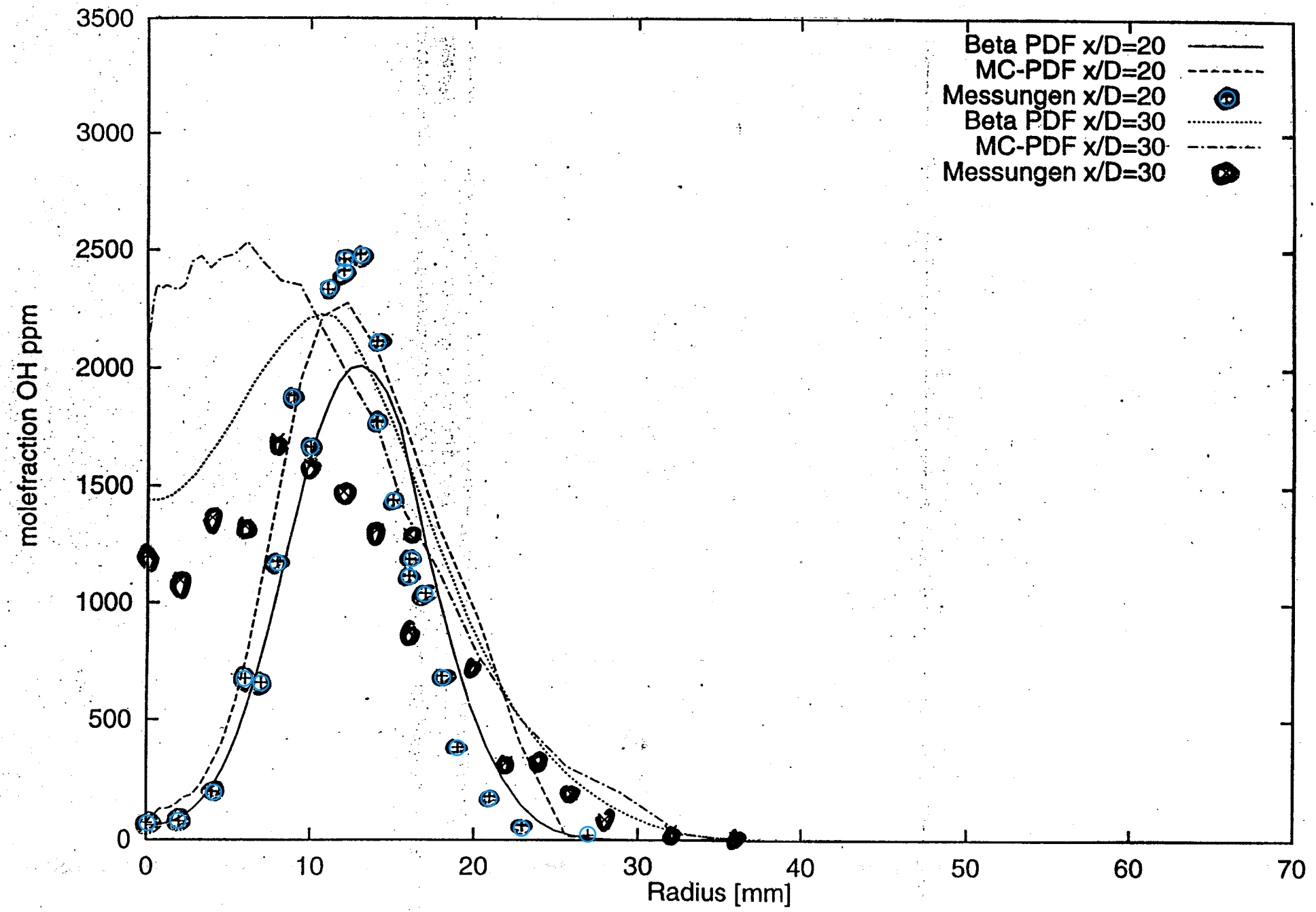
# Pure H2 Jet flame: PDF +5step CCOr=0.02+r+g

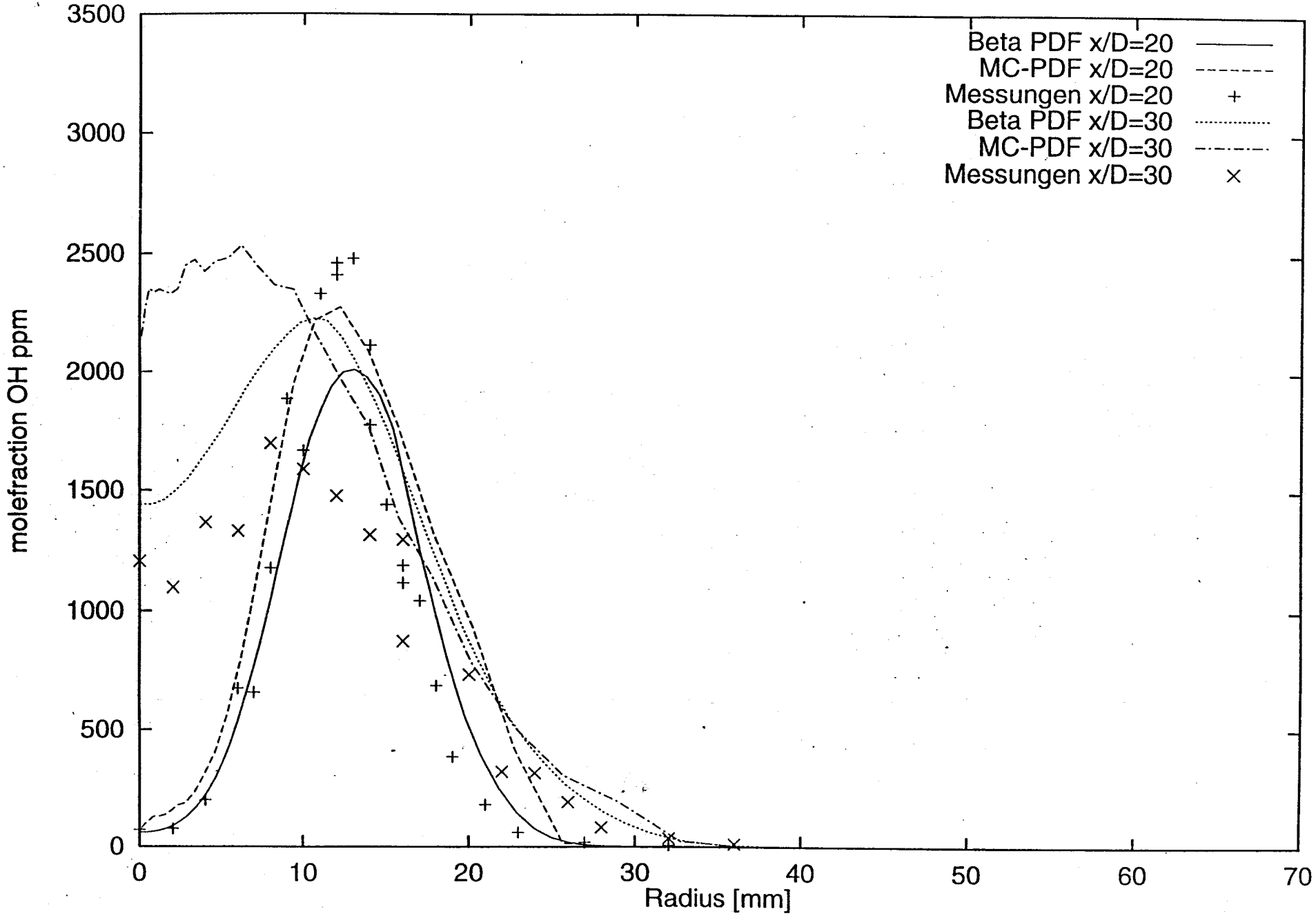


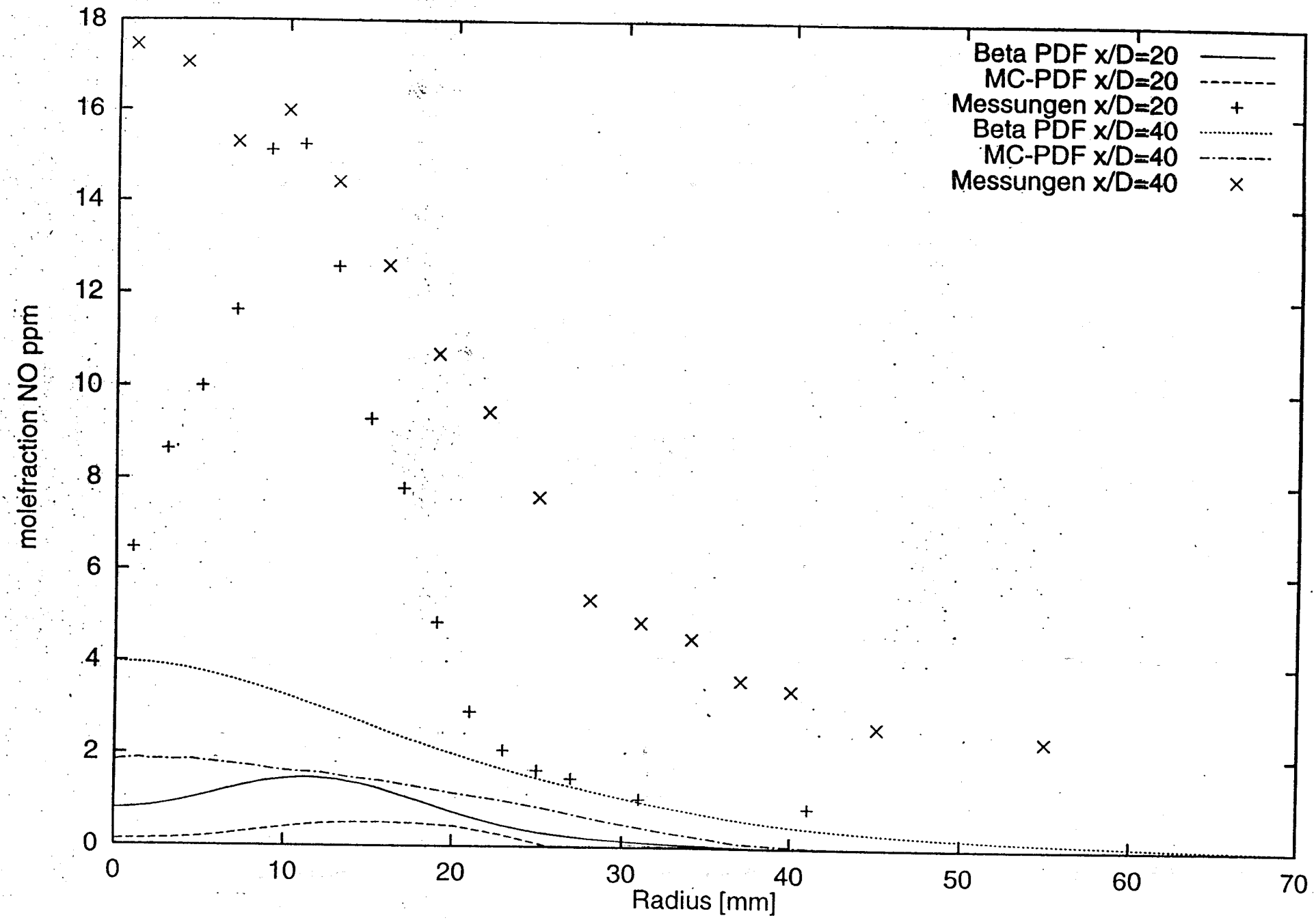

Beta-PDF (THD)
Lagr.-PDF (THD)
Euler-PDF (UCB)
Raman Data (THD)
Centerline Mixture Fraction -f-
Normalized Axial Downstream Position -x/D-
0
0.2
0.4
0.6
0.8
1
0
10
20
30
40
50
60
70

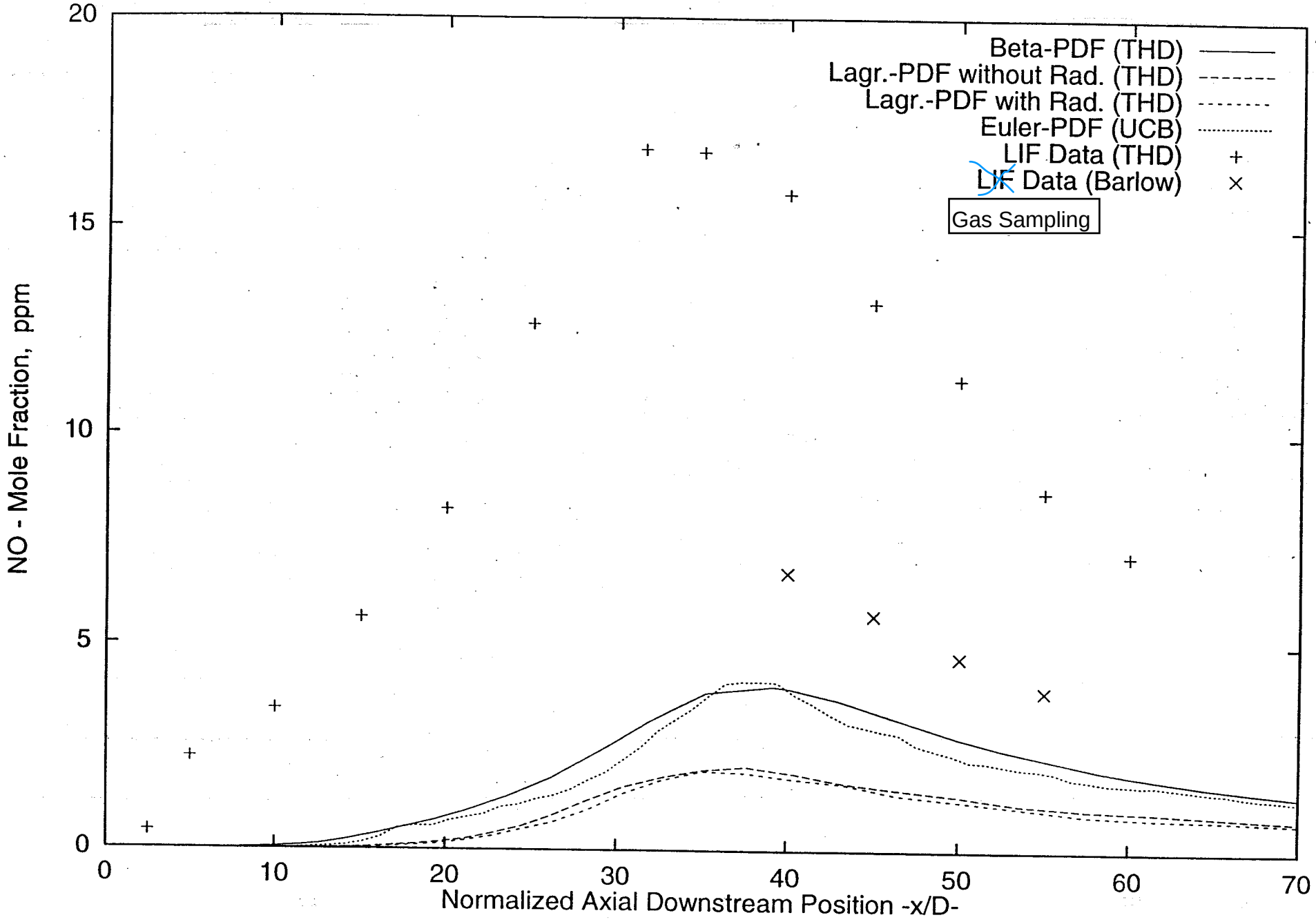

Beta-PDF x/D=20
MC-PDF x/D=20
Messungen x/D=20
Beta-PDF x/D=30
MC-PDF x/D=30
Messungen x/D=30
Temperatur [K]
Radius [mm]
0
500
1000
1500
2000
0
10
20
30
40
50
60
70


Beta-PDF (THD)
Beta-PDF Equil. (THD)
Lagr.-PDF without Rad. (THD)
Lagr.-PDF with Rad. (THD)
Euler-PDF (UCB)
LIF Data (THD)
OH - Mole Fraction, ppm
Normalized Axial Downstream Position -x/D-
0
500
1000
1500
2000
2500
3000
0
10
20
30
40
50
60
70

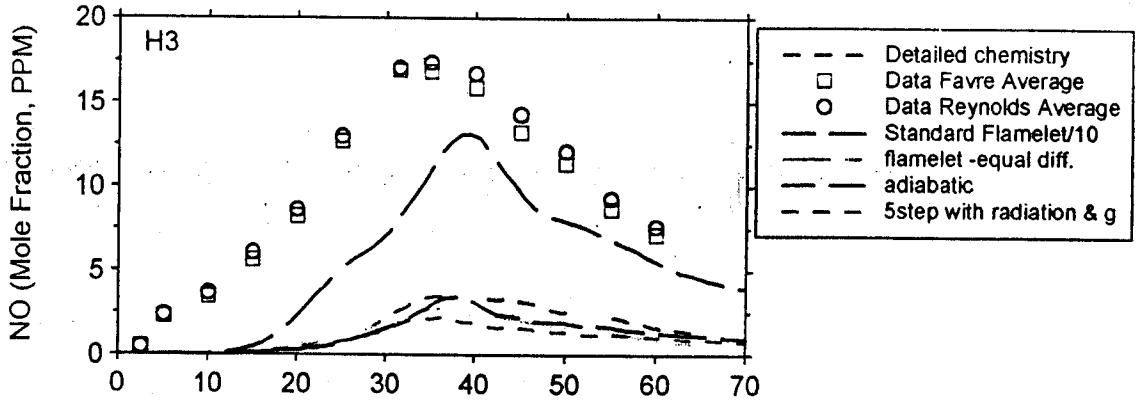

Beta PDF x/D=20
MC-PDF x/D=20
Messungen x/D=20
Beta PDF x/D=30
MC-PDF x/D=30
Messungen x/D=30
molefraction OH ppm
Radius [mm]
0
500
1000
1500
2000
2500
3000
3500
0
10
20
30
40
50
60
70

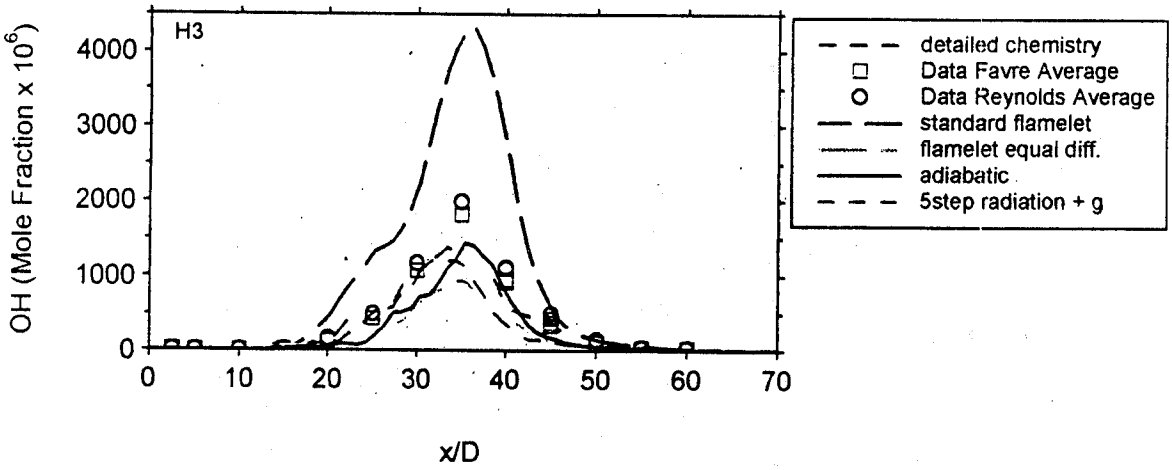

Beta PDF x/D=20
MC-PDF x/D=20
Messungen x/D=20
Beta PDF x/D=30
MC-PDF x/D=30
Messungen x/D=30
molefraction OH ppm
Radius [mm]
0
500
1000
1500
2000
2500
3000
3500
0
10
20
30
40
50
60
70


Beta PDF x/D=20
MC-PDF x/D=20
Messungen x/D=20
Beta PDF x/D=40
MC-PDF x/D=40
Messungen x/D=40
molefraction NO ppm
Radius [mm]
0
2
4
6
8
10
12
14
16
18
0
10
20
30
40
50
60
70


Beta-PDF (THD)
Lagr.-PDF without Rad. (THD)
Lagr.-PDF with Rad. (THD)
Euler-PDF (UCB)
LIF Data (THD)
LIF Data (Barlow)
Gas Sampling
NO - Mole Fraction, ppm
Normalized Axial Downstream Position -x/D-
0
5
10
15
20
0
10
20
30
40
50
60
70

# Comparison of Predictions with Experimental Data Turbulent 50%$H_2$+50%$N_2$ Jet Flame (H3)



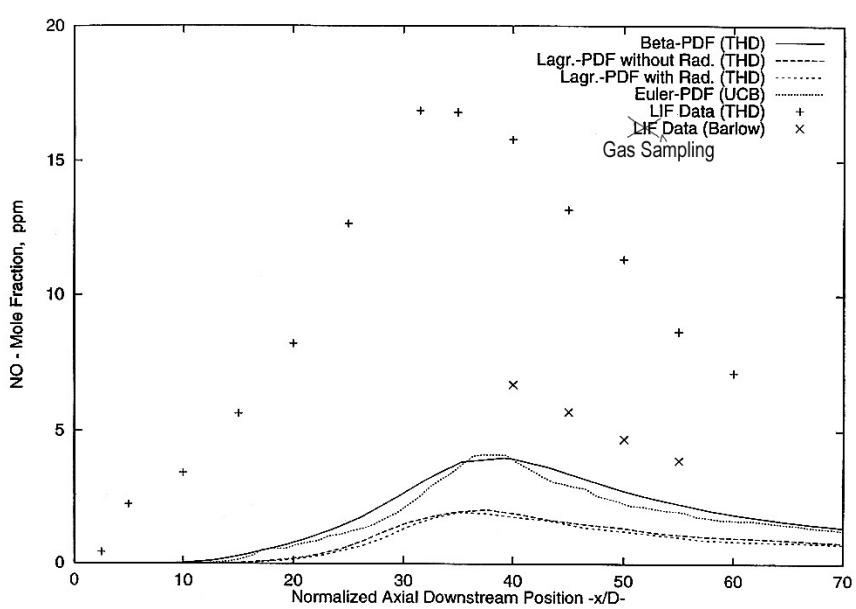
# Retrospective Comments on NO Comparisons in $H_2$ Jet Flames

R. S. Barlow – January 2003

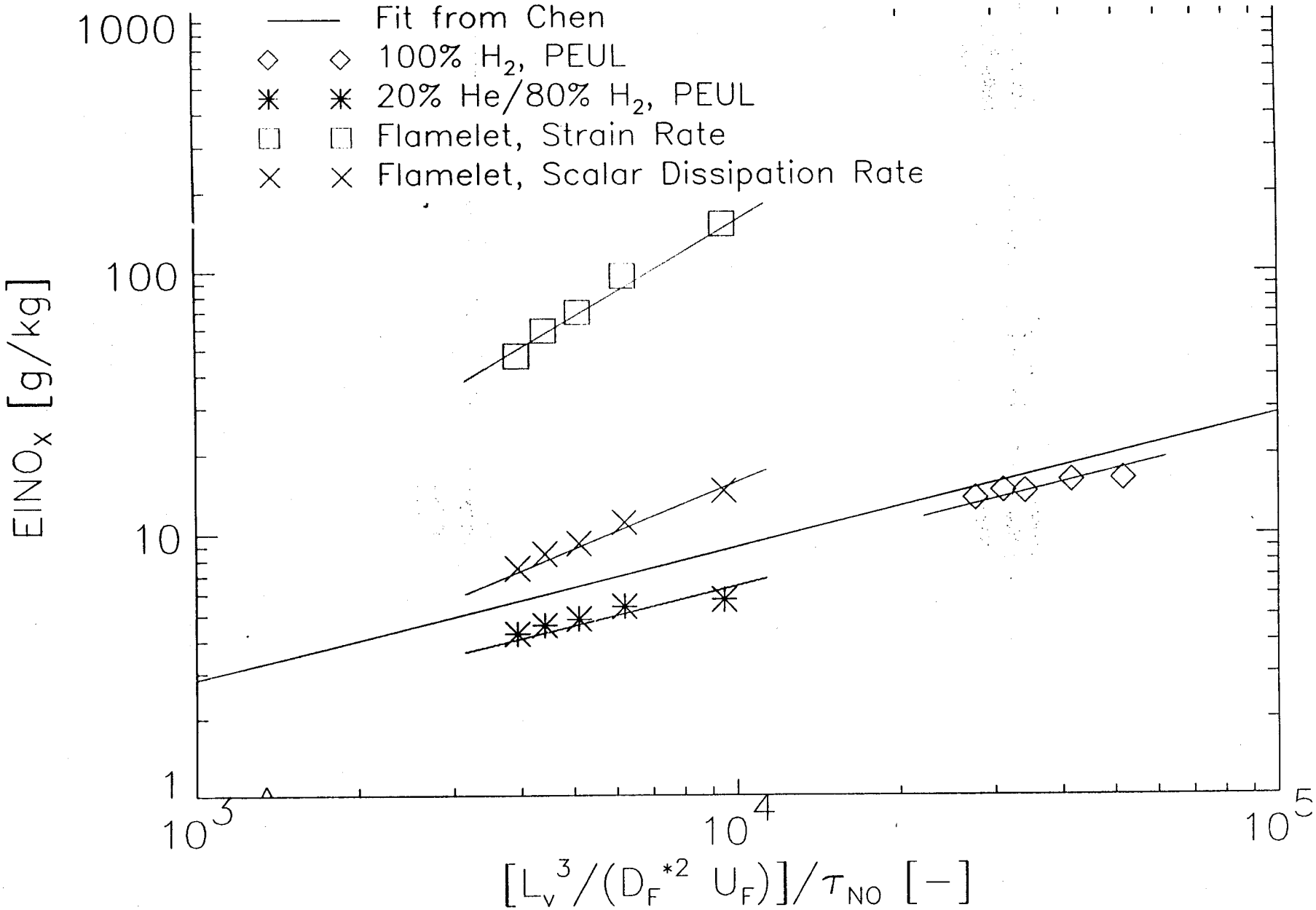
During preparations for TNF2 comparisons of measured and modeled results for simple $H_2$ jet flame, discrepancies were noted in the relative NO predictions for the TU Darmstadt and Sandia flames. Specifically, the ratio of measured NO to predicted NO from J-Y Chen's pdf calculations was significantly higher in the Darmstadt H3 flame than in the Sandia $H_2$/He flames. This was considered as a possible indication of inconsistency between NO measurements from the two labs. In order to shed light on this issue, probe-sampling measurements were conducted in the TDF lab (R. S. Barlow and J. H. Frank, May 1997, unpublished data). Measurements included NO, $O_2$, and $CO_2$. Samples were extracted using a quartz probe and heated line. The NO measurements were calibrated using sample gases with known NO concentration diluted in $N_2$. NO measurements were then performed in the following flows and flames:

- McKenna burner, premixed $CH_4/O_2/N_2$ undoped and with amounts of NO-doped $N_2$ replacing the undoped $N_2$. These are the same flames used to calibrate the NO LIF measurements at Sandia. Cold flows with air plus NO/$N_2$ were also sampled.
- TU Darmstadt H3 flame at x/d=40, 45, 50, 55 on the centerline.
- Sandia $H_2$ flame with 40% He dilution at x/d=100 (x=L_vis) on the centerline.

NO sampling calibration results in cold gases and flat calibration flames were consistent within +/- 10 percent. NO sampling results in the Sandia $H_2$/He flame were in agreement within 12 percent (12.6 ppm from the laser measurements, and 11.3 ppm from sampling). Sampling probe measurements of NO were significantly lower than laser measurements reported by TU Darmstadt for the H3 flame. This comparison was made at TNF2 and is shown below (see also p. 52). The discrepancy may be associated with NO LIF calibration procedure used for the TU Darmstadt measurements. This possibility was discussed at TNF2 but has not been confirmed.



# EINOX Scaling

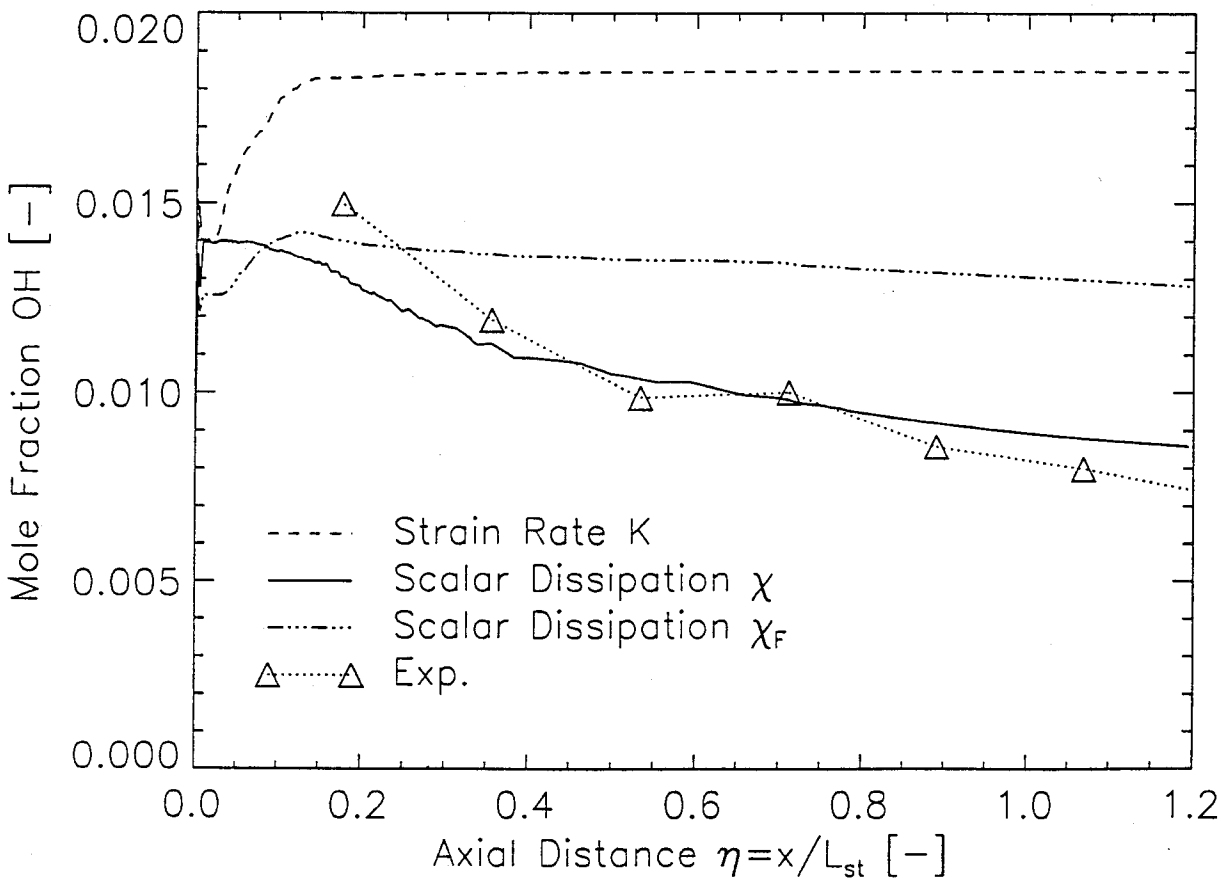


# Coupling between Turbulent Flow and Flamelet Library

$$\tilde{K} = C_K \frac{\tilde{\varepsilon}}{\tilde{k}}$$

$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{Z''^2}$$

$$\tilde{\chi}_F = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} (\Delta Z_F)^2$$

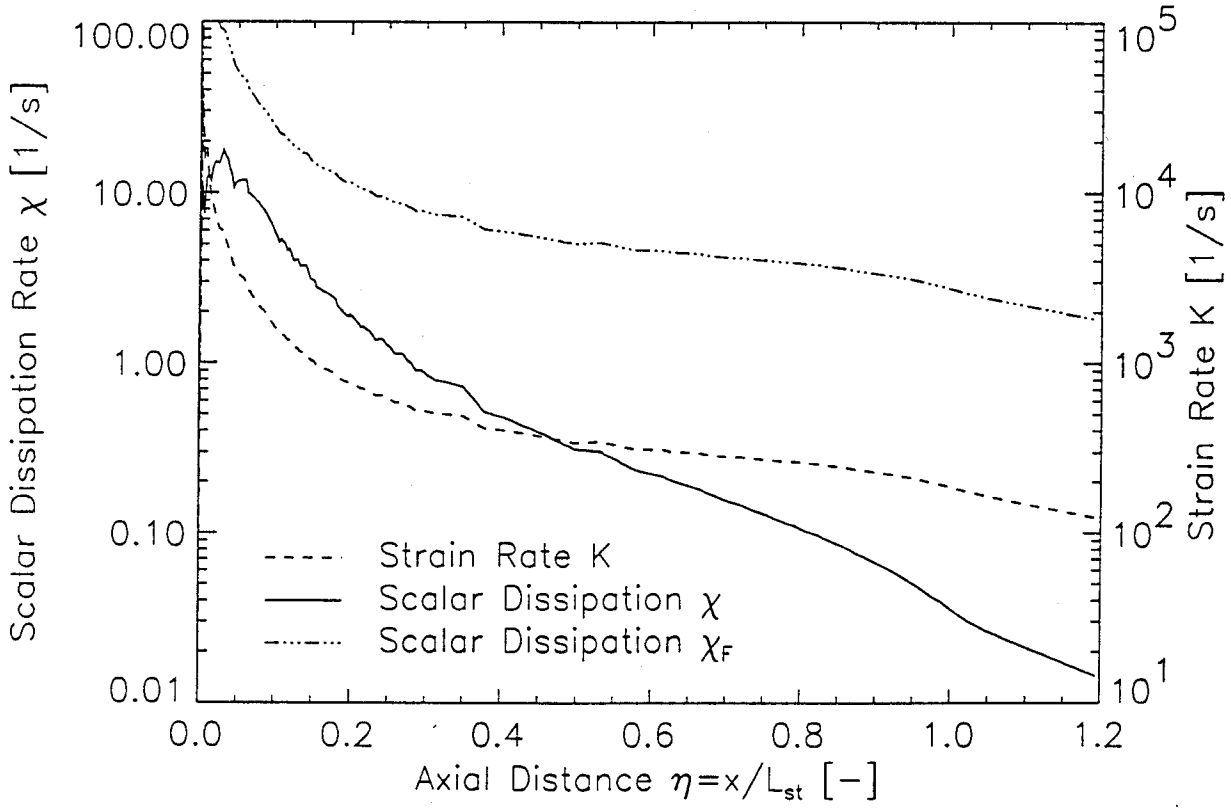


# Coupling between Turbulent Flow and Flamelet Library

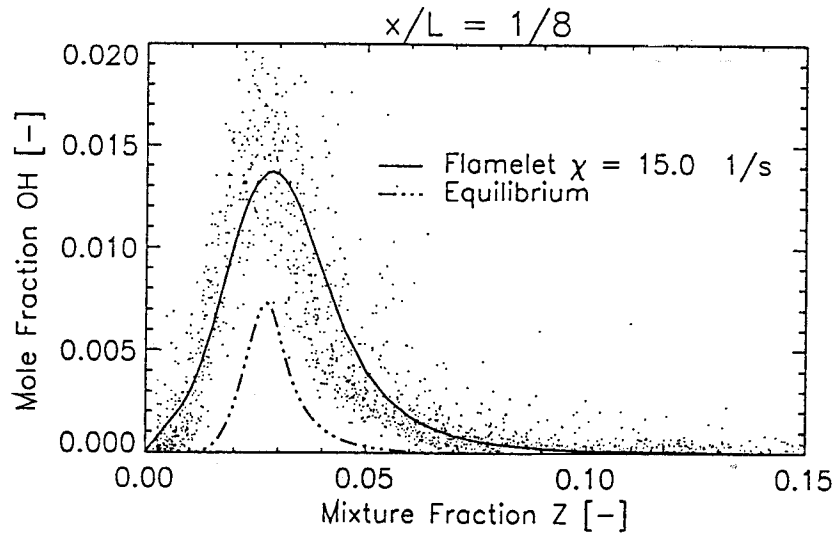
$$\tilde{K} = C_K \frac{\tilde{\varepsilon}}{\tilde{k}}$$

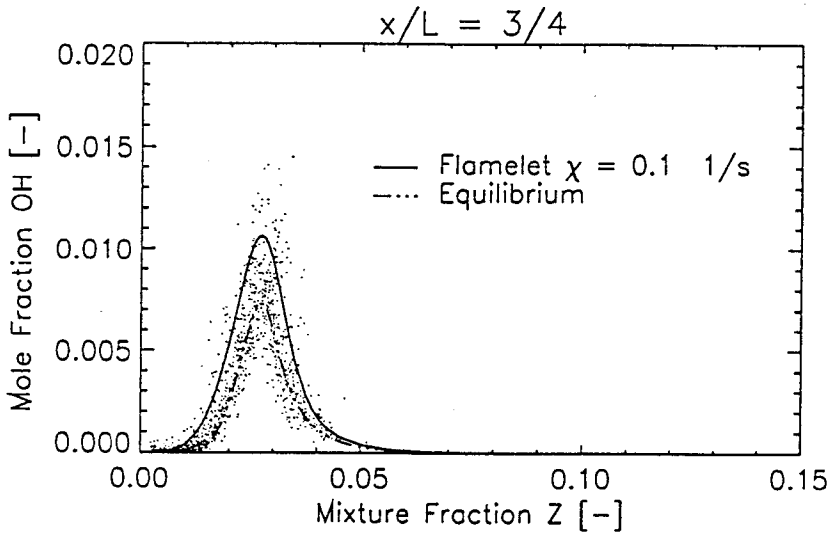
$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{Z''^2}$$

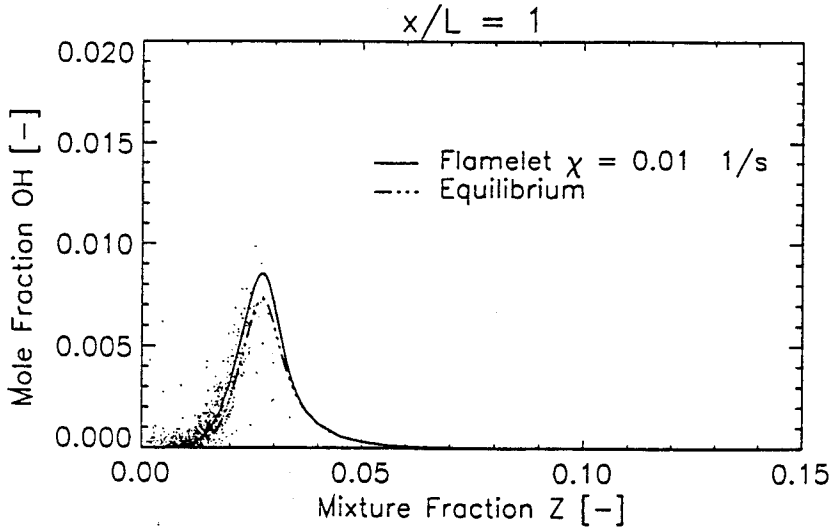
$$\tilde{\chi}_F = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} (\Delta Z_F)^2$$



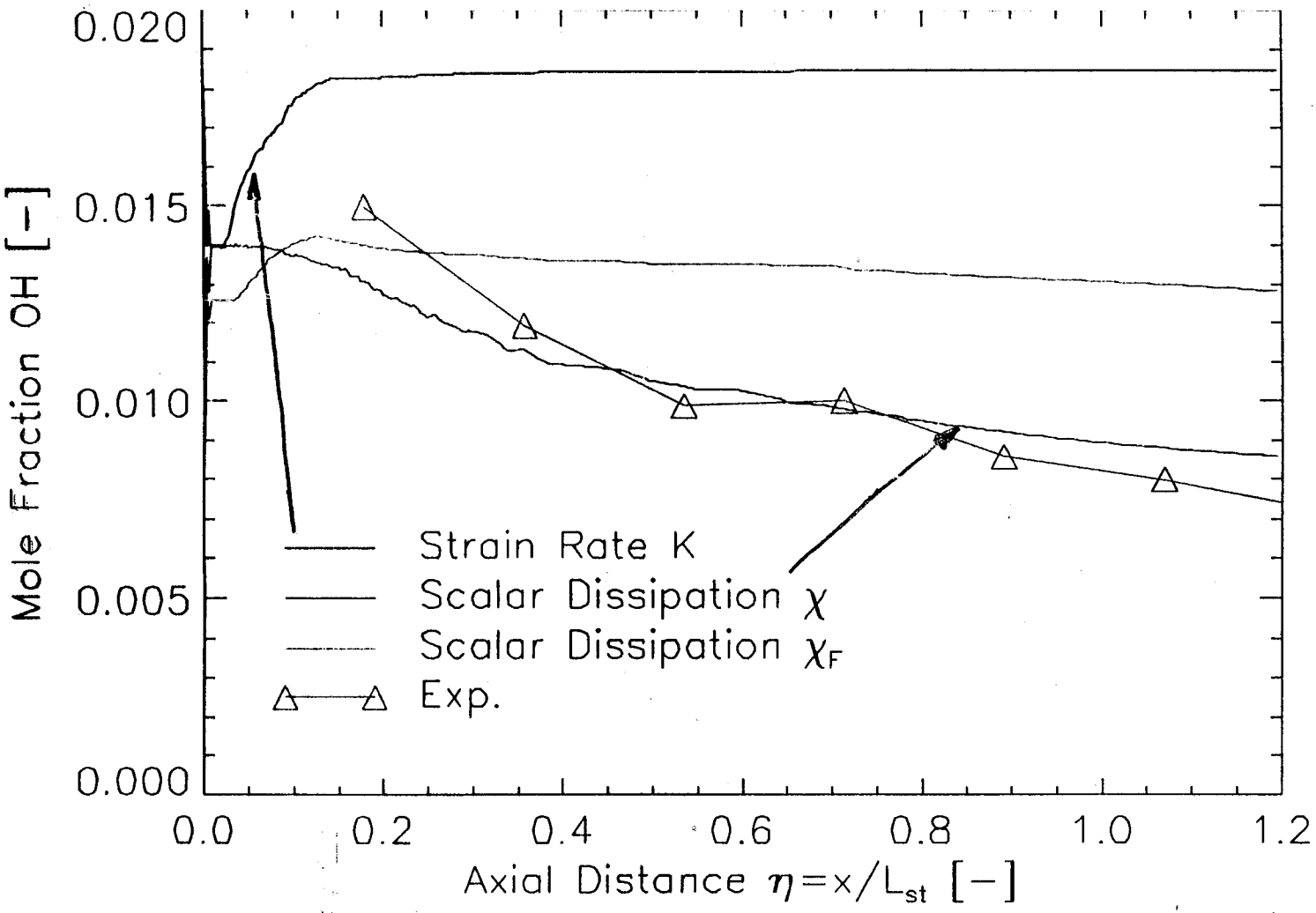
# Scatter Plotts OH



# OH at Stochiometric Mixture Fraction

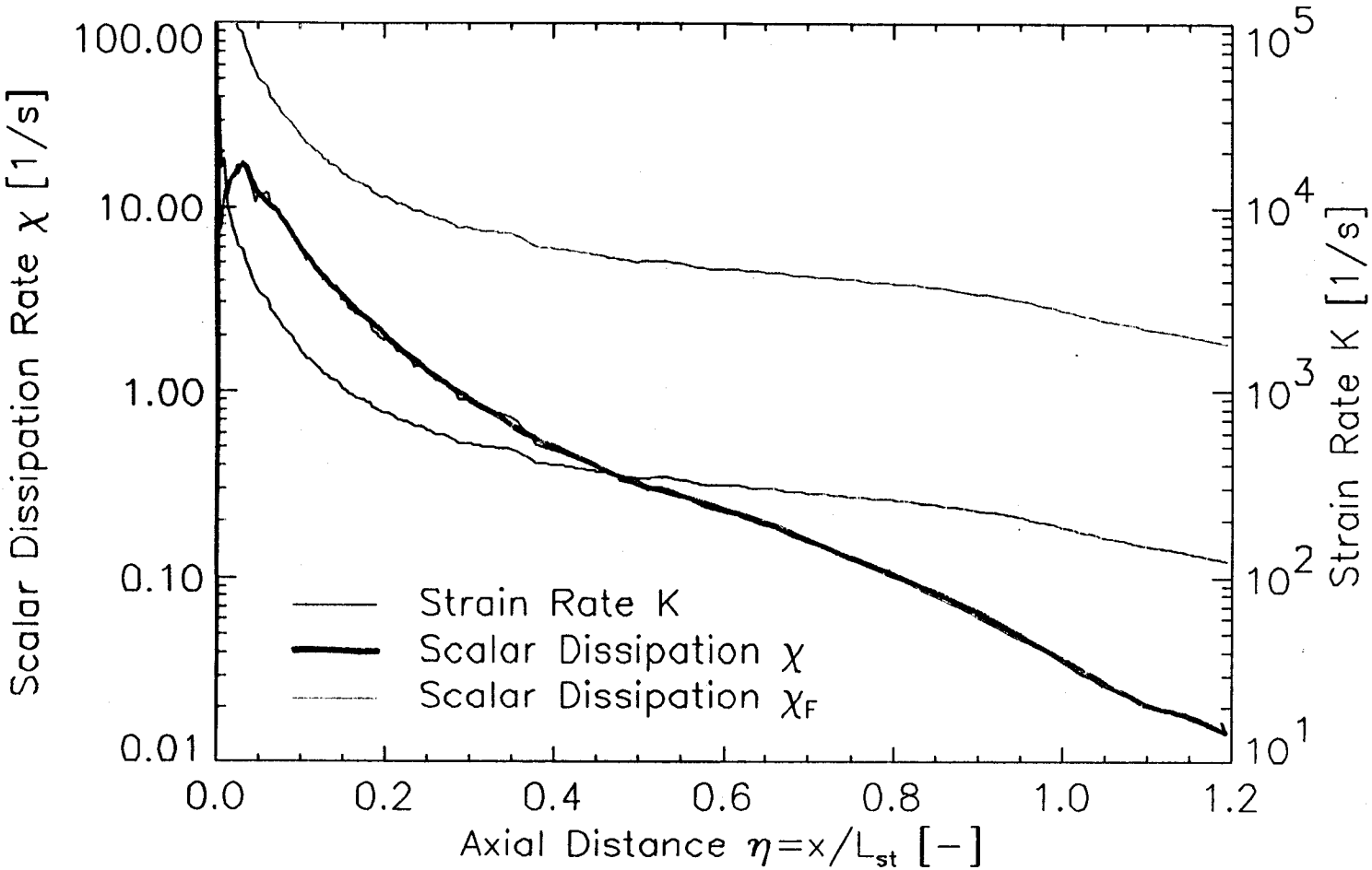



$$\tilde{K} = C_K \frac{\tilde{\varepsilon}}{\tilde{k}}$$

$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{Z''^2}$$

$$\tilde{\chi}_F = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} (\Delta Z_F)^2$$

# $\tilde{K}$ and $\tilde{\chi}$ at Stochiometric Mixture Fraction

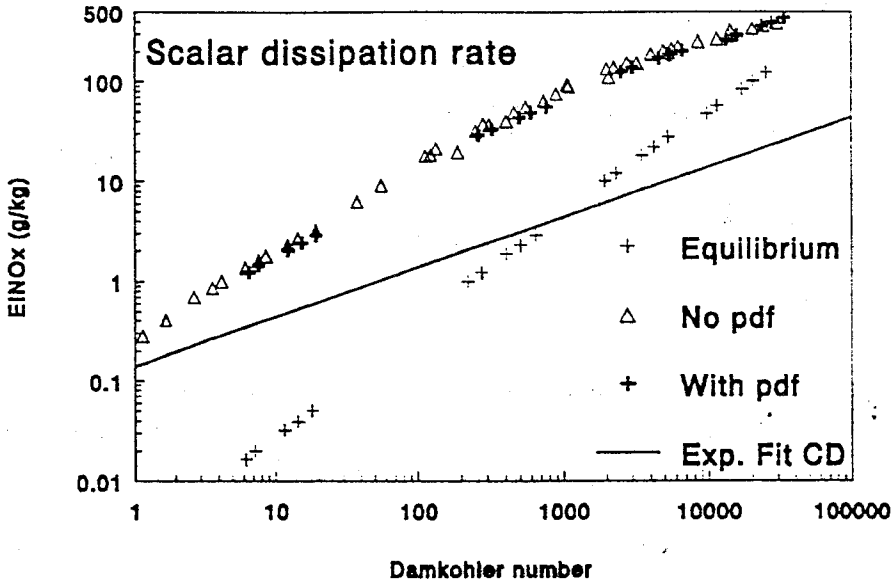



$$\tilde{K} = C_K \frac{\tilde{\varepsilon}}{\tilde{k}}$$

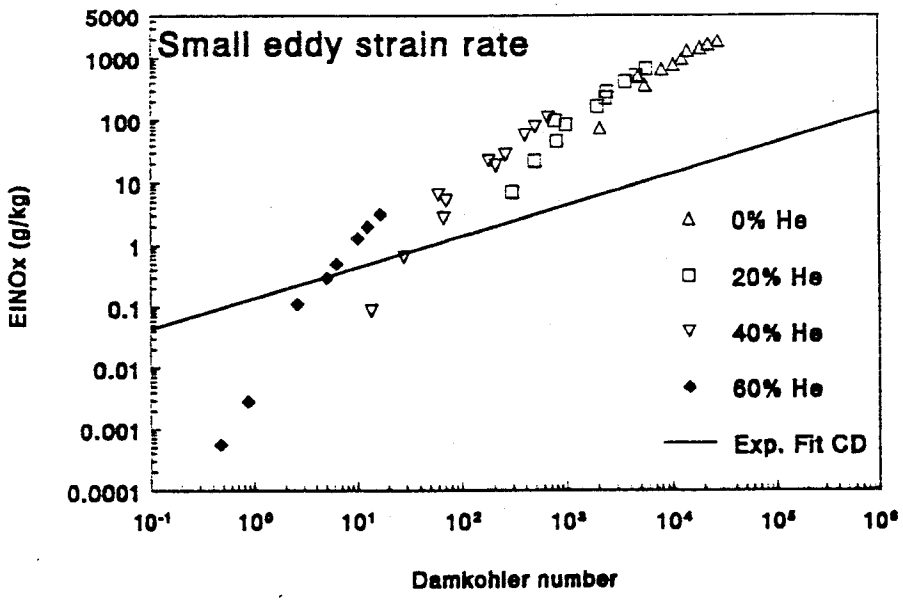
$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{Z''^2}$$

$$\tilde{\chi}_F = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} (\Delta Z_F)^2$$

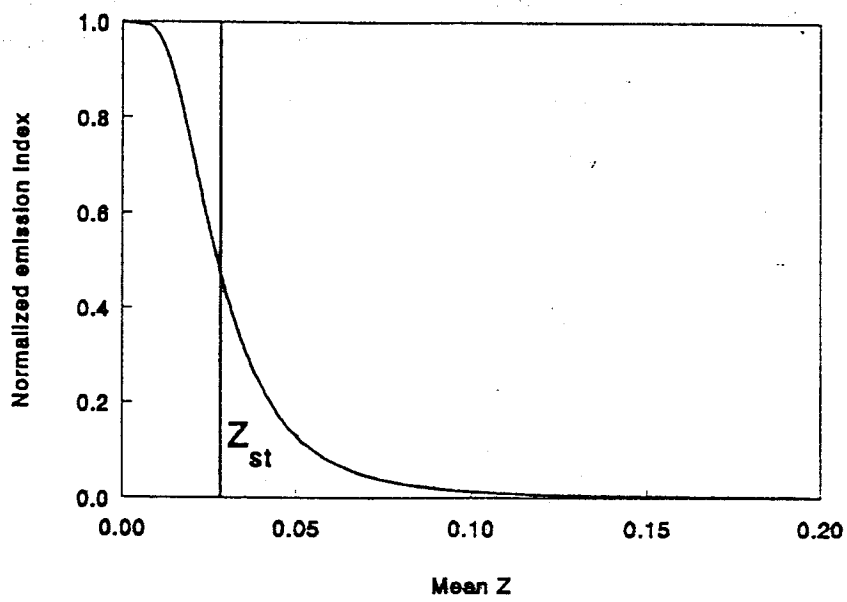
Sanders




*$EINO_x$ vs $Da$ number predicted with the scalar dissipation rate.*



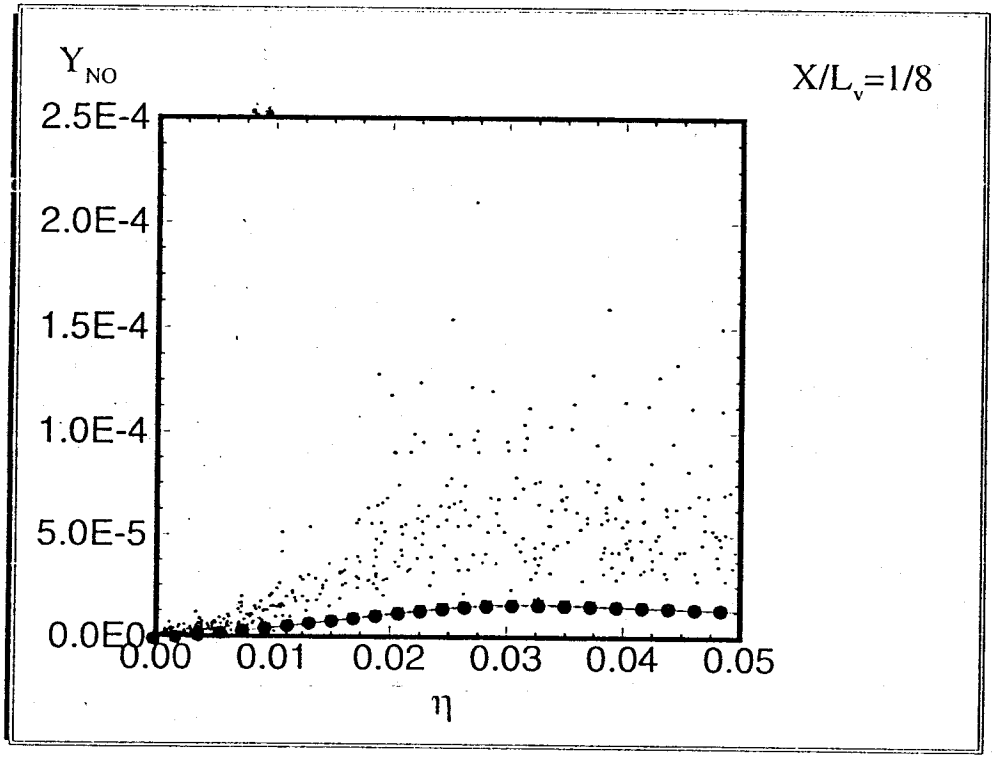

*$EINO_x$ vs $Da$ number predicted with the small eddy strain rate.*

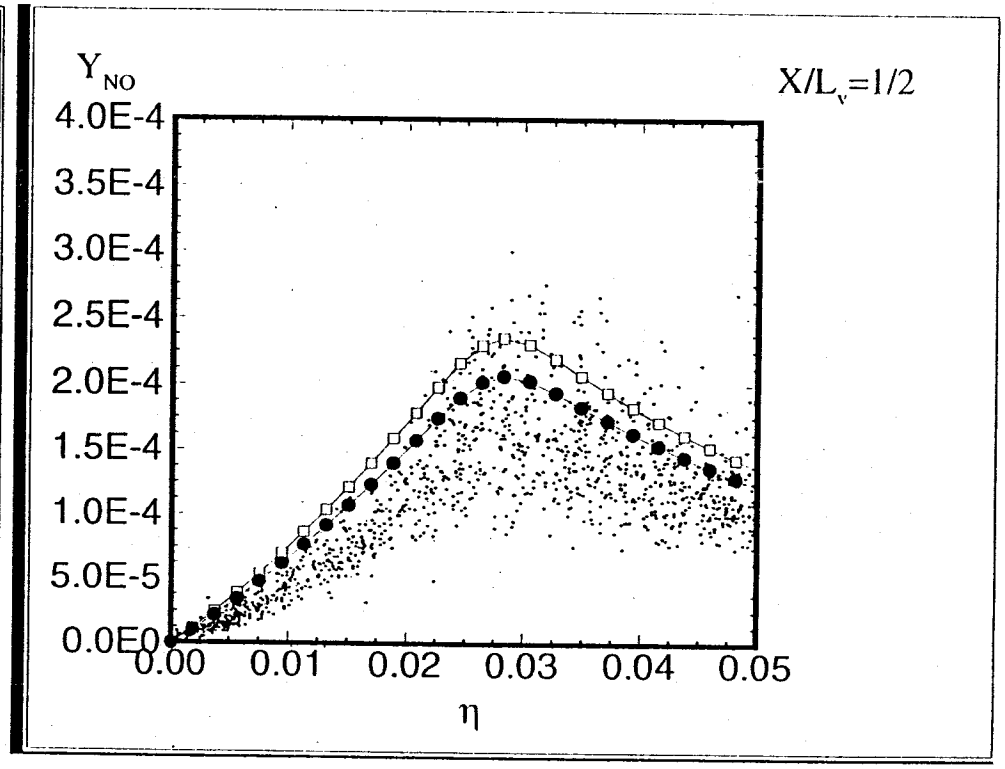



*'Partial' emission index $EINO_x(x)$ in a turbulent flame*

Main contribution from $\tilde{Z}_c \approx Z_{st}$

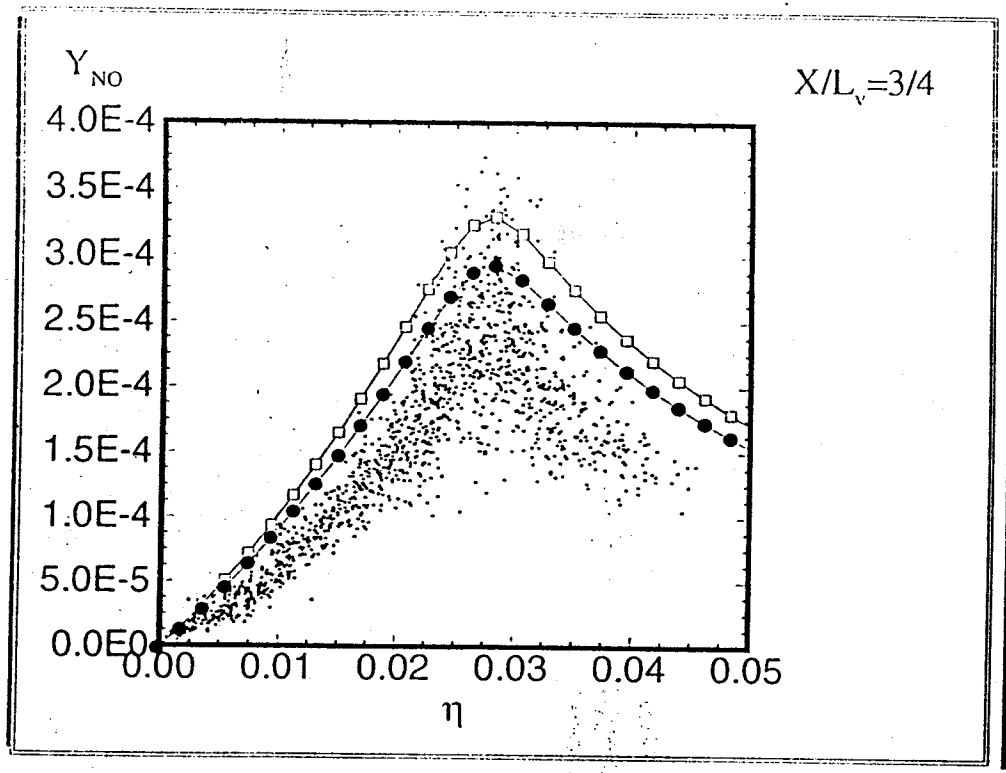
# NO predictions

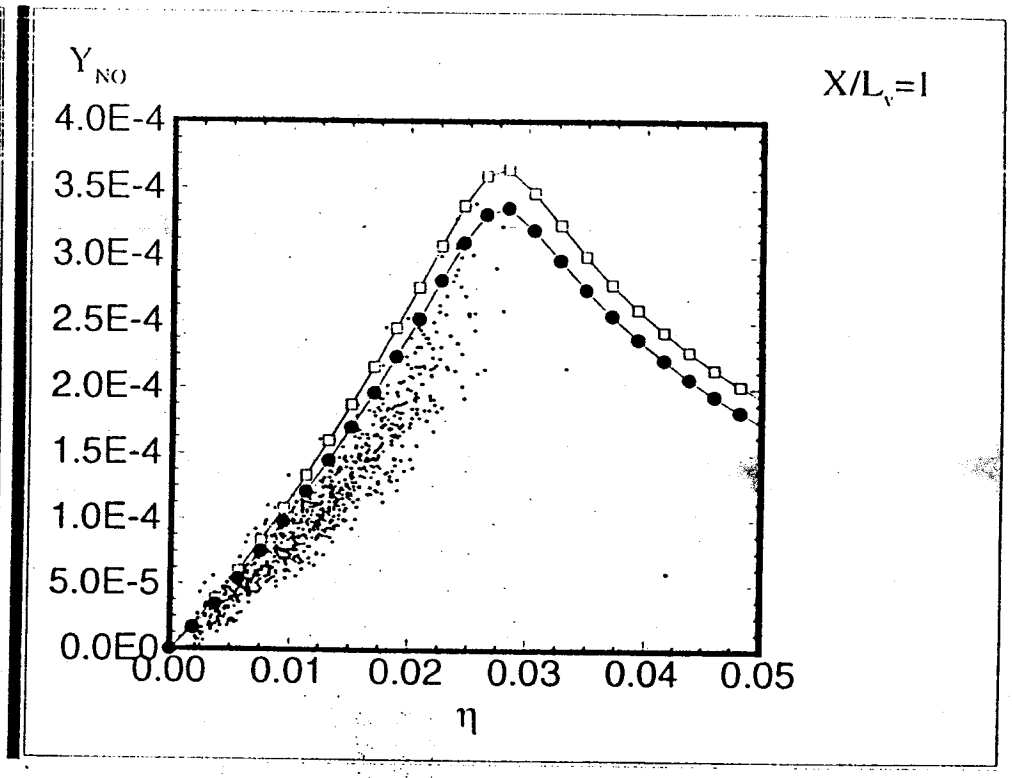



NO predictions at different downstream locations: 2nd order closure (circles), 1st order closure (squares), experimental data (dots).

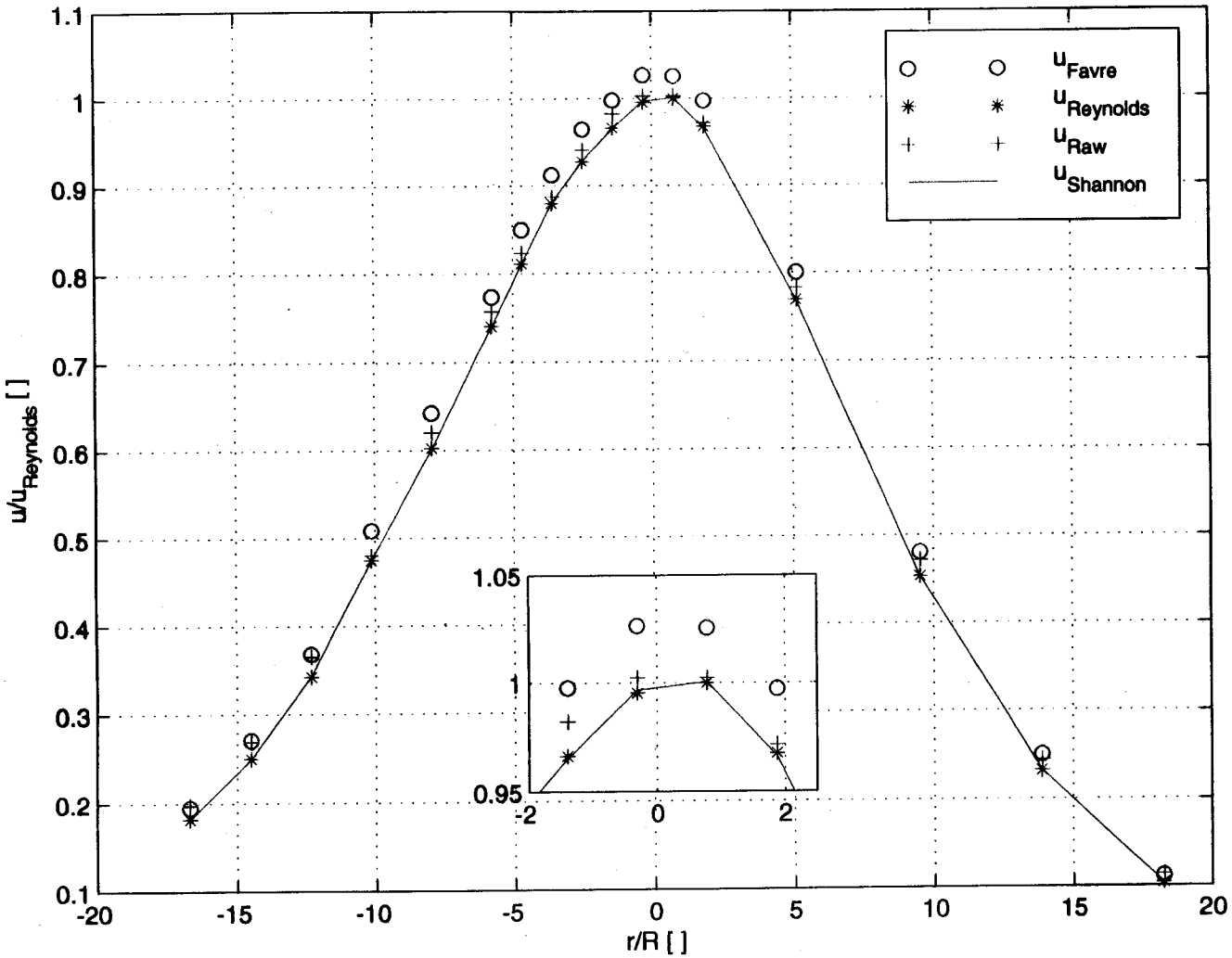
# NO Predictions




NO predictions at different downstream locations: 2nd order closure (circles), 1st order closure (squares), experimental data (dots).

# Differences betwwen Reynolds and Favre Averaged Mean Velocities at the 40%/30%/30% $CO/H_2/N_2$ Flame. Is LDV Favre Averaged ?




At x/D = 60 the specific gas constant R is constant over the radius. Therefore the density of the gas is only a function of the temperature.
With the coincident measurements of the temparature and the velocity the Favre average could be calculated.

# FLAME RADIATION

# MEASUREMENTS AND MODELS

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**School of Mechanical Engineering**
**Purdue University**
**West Lafayette, IN 47907**

- **NIST and NSF have supported the author's work in radiation.**

- **Thanks to Rob Barlow for asking the questions that led to this presentation.**

- **Thanks to Darmstadt group for organization and hospitality.**

# Background

- **Interest in thermal radiation has traditionally been for heat flux to surrounding objects.**

- **Effects on kinetics of pollutant species such as NO and soot have renewed the interest and brought new challenges and questions for example: 5% energy loss from $H_2$/air flame has big effect on $N_2 \rightarrow$ NO chemistry.**

# What to Measure?

- **When we need $\dot{\omega}_i'''$ information, we typically make do with $Y_i$ measurements.**
- **If we need $\dot{Q}_{Rad}'''$ information, analogous information is provided by $Y_i$ and T measurements.**
- **Energy equation can be written as:**

$$\rho\frac{\partial H}{\partial t}+\rho\vec{V}\cdot\nabla H=\nabla\cdot\rho\alpha\nabla H-\dot{Q}_{Rad}'''$$

$$H=\Sigma Y_i\left(h_{fi}^{o}+\int_{T_{\mathrm{Re}f}}^{T}C_{pi}dT\right)$$

**Or as:**

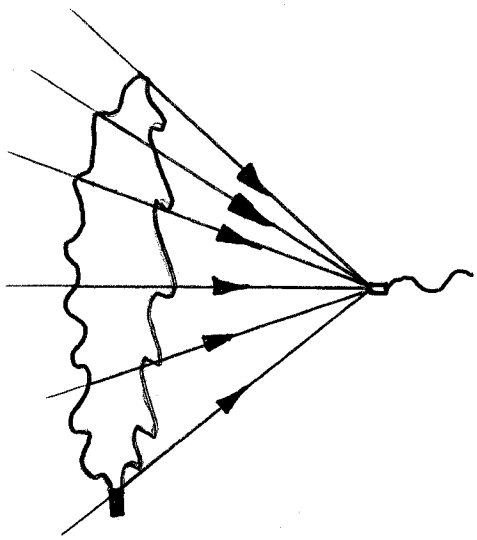
$$\rho Cp_m\frac{\partial T}{\partial t}+\rho Cp\vec{V}\cdot\nabla T=\nabla\cdot\lambda\nabla T+\left(-\Sigma h_{fi}^{o}\dot{\omega}_i'''\right)-\dot{Q}_{Rad}'''$$

$$\rho\frac{\partial Y_i}{\partial t}+\rho\vec{V}\cdot\nabla Y_i=\nabla\cdot\rho D\nabla Y_i+\dot{\omega}_i'''$$

**If transient species and temperature distributions including their various derivatives are known then $\dot{Q}_{Rad}'''$ can be obtained from the above equations.**

# Radiation Measurements

**Opportunity to measure the direct effect of $\dot{Q}''''_{Rad}$ by measuring radiation to environment. (Similar to species emission index measurements)**



- **Heat flux at detector is related to cumulative effect of radiative heat loss (exchange) at multiple points along the line of sight.**

- $H_2O$ **Radiation is highly spectral.**

- **Limiting optics can be used to isolate narrow view angle paths.**

# Heat Flux Detector

- Wide view angle (150° detectors are available)
- Positioning: Emitting parts of the flame should not be in blind spots (15° to surface)
- Detector must have high absorptivity and must be spectrally flat. Windows (Sapphire, $CaF_2$, ZnSe, ZnS) have complicated matters in past data since $H_2O$ has bands up to 200 μm.
- Direct calibration is not trivial
- Limited view angle calibration is feasible.

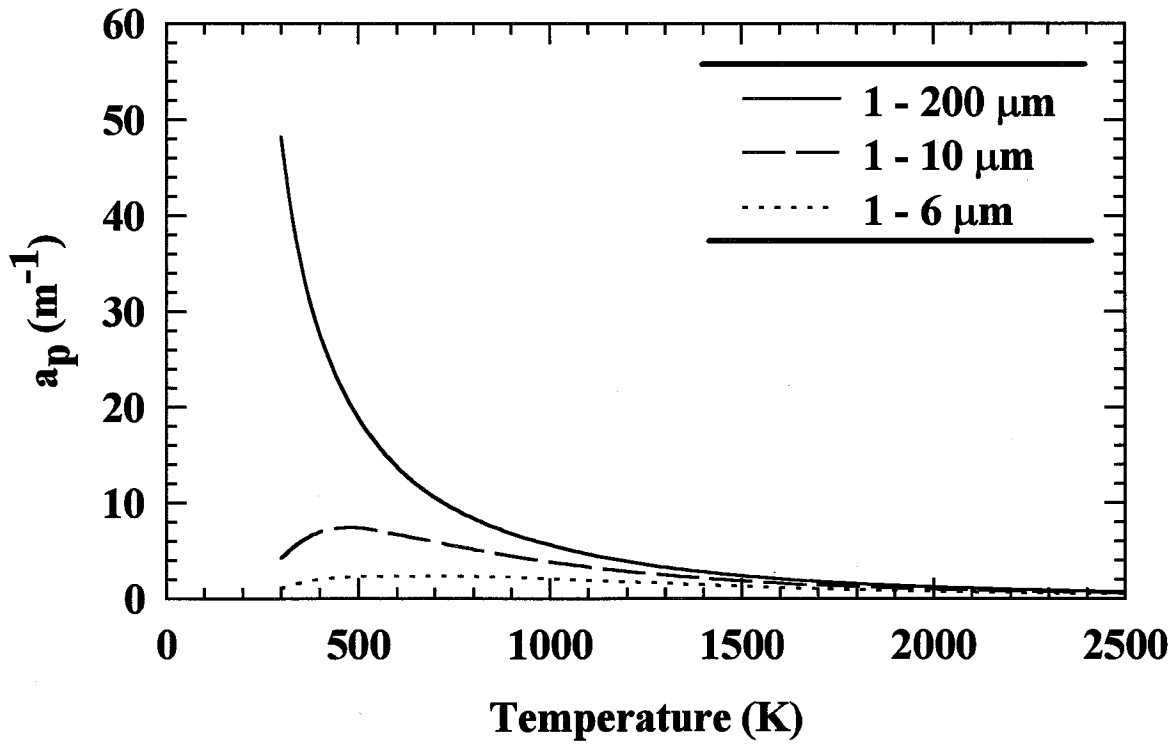
## Detector Windows

- Since water has many bands (1.38, 1.87, 2.7, 6.3 and 71 microns) and these bands are broadened significantly, use of a spectrally flat wide band detector is necessary.

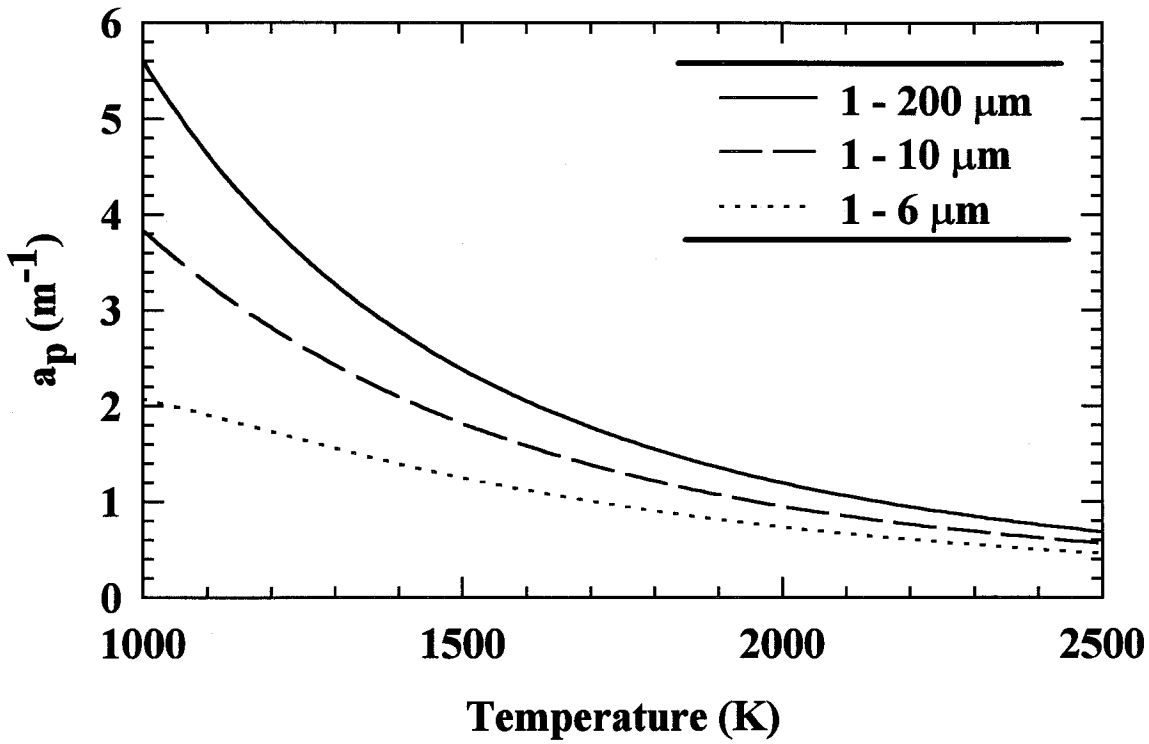
- We had problem interpreting our heat flux data in our 1987 (Gore et al.) work because of the wavelength cutoff of our sapphire window.

- Manufacturer's calibrations can vary between 10% to 20% (Sample size 6 detectors between 1987-1993)

- NIST has a new heat flux standard test method and master detector.




**Planck mean absorption coefficient for water vapor.**




**Planck mean absorption coefficient for water vapor.**

## Modeling

$$\rho \frac{\partial H}{\partial t} + \rho \vec{V} \cdot \nabla H = \nabla \cdot \rho \alpha \nabla H - \dot{Q}'''_{emitted} + \dot{Q}'''_{absorbed}$$

## Non-dimensional Numbers

**If optically thin**

$$\Pi_e = \frac{\dot{Q}'''_{emitted} L_{ch}}{\rho_{ch} V_{ch} H_{ch}} = \frac{4 a P_{ch} \sigma T_{ch}^3 L_{ch}}{\rho_{ch} V_{ch} Cp_{ch}}$$

≡Emission Number

- **If emission number is large ~ 1 then radiation affects energy balance.**
- **Recent excitement is because even small emission numbers are affecting chemistry significantly. Ratio of activation temperature for specific reactions and characteristic temperature with and without radiation is relevant!**

## Absorption Number

$$\Pi_a = \frac{\dot{Q}''' _{absorbed} L_{ch}}{\rho_{ch} V_{ch} H_{ch}} = \frac{4 a_i \Pi \bar{i}_i L_{ch}}{\rho_{ch} V_{ch} Cp_{ch} T_{ch}}$$

**Most modeling efforts are currently neglecting $\Pi_a$ stating that $\int a_p x_{H_2O} ds$ is small. The proper quantity to examine is the ratio of $\Pi_a$ and $\Pi_e$**

$$\Pi_{ae} = \frac{a_i \Pi \bar{i}_i}{a p_{ch} \sigma T_{ch}^4}$$

**For our $H_2$ /air flames $\Pi_{ae}$ is 0.1 to 0.2 → source of maximum 20% error.**

## Optically thin assumption

$$\frac{di_\lambda}{ds} = -a_\lambda i_\lambda + a_\lambda i_{\lambda b}$$

**Volumetric energy loss by emission**

$$\dot{Q}''' _{emitted} = \frac{4\Pi}{\Delta S}\int_o^\infty \left(1 - \bar{e}^{\int_o^{\Delta s} a_\lambda ds}\right) i_{\lambda b} d_\lambda$$

**If** $\int_o^{\Delta s} a_\lambda ds$ **is small then**

$$= \frac{4\Pi}{\Delta s}\int_o^\infty \{1 - 1 + a_\lambda \Delta s \ldots\} i_{\lambda b} d\lambda$$

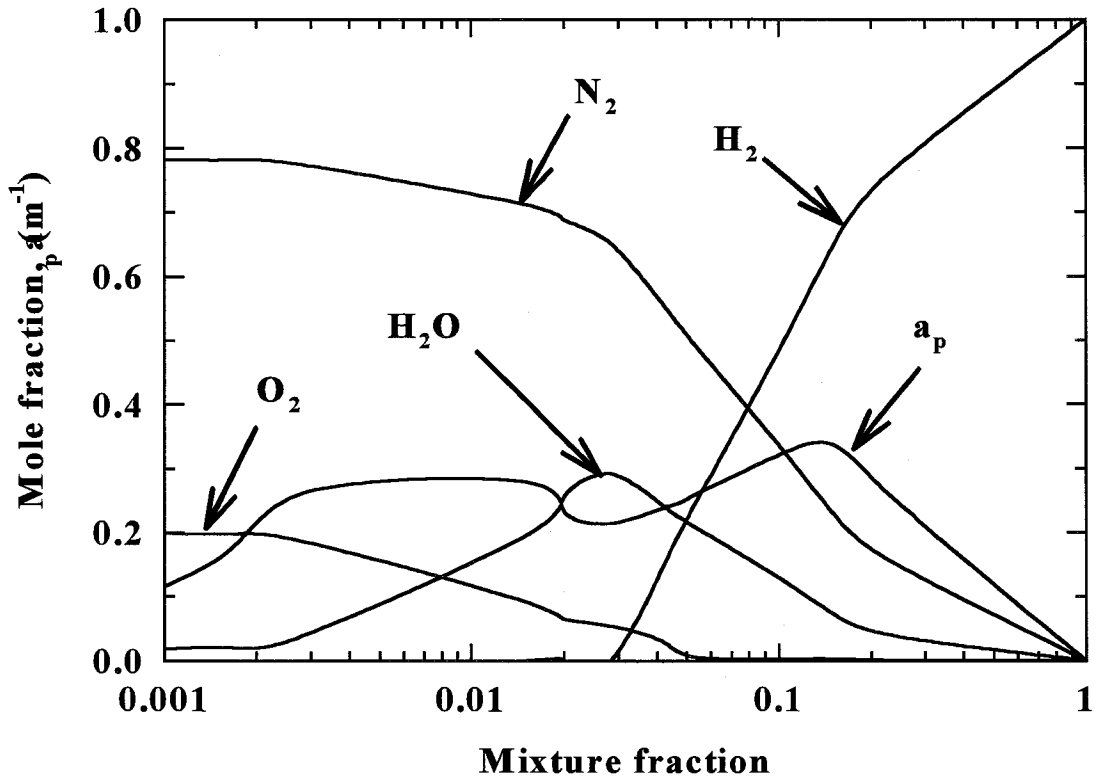
$$= 4\Pi \int_o^\infty a_\lambda i_{\lambda b} d\lambda = 4\Pi a_p X_{H_2O} \frac{\sigma T^4}{\Pi}$$

$$= 4 a_p X_{H_2O} \sigma T^4$$

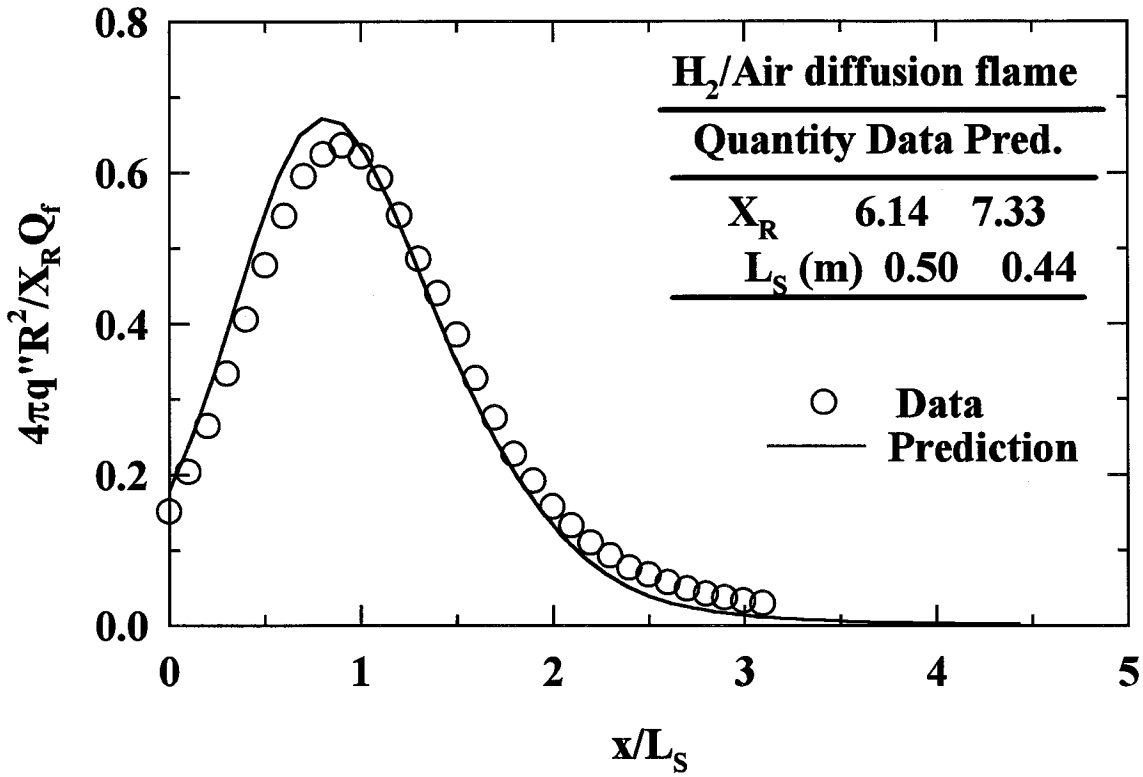
**(Optically thin assumption is independent of emission only assumption)**

## An Example

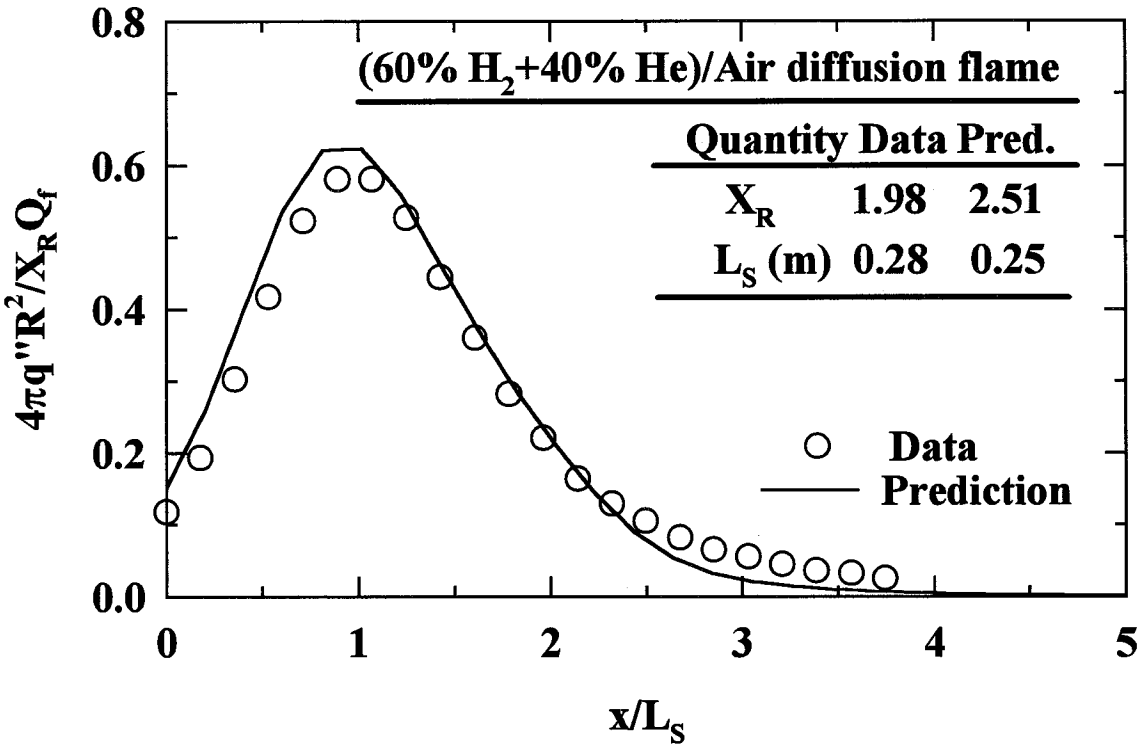
- **Sandia Flame 1: $H_2$/air**
- **Laminar flamelet state-relations for species and $a_P$ used. T calculated locally.**
- **Measurements in collaboration with Dr. Barlow with 1 - 6.3 μm cutoff windows.**
- **Radiation predictions are favorable.**
- **NO predictions are sensitive to $O_2$ in addition to T state-relations do not work well.**



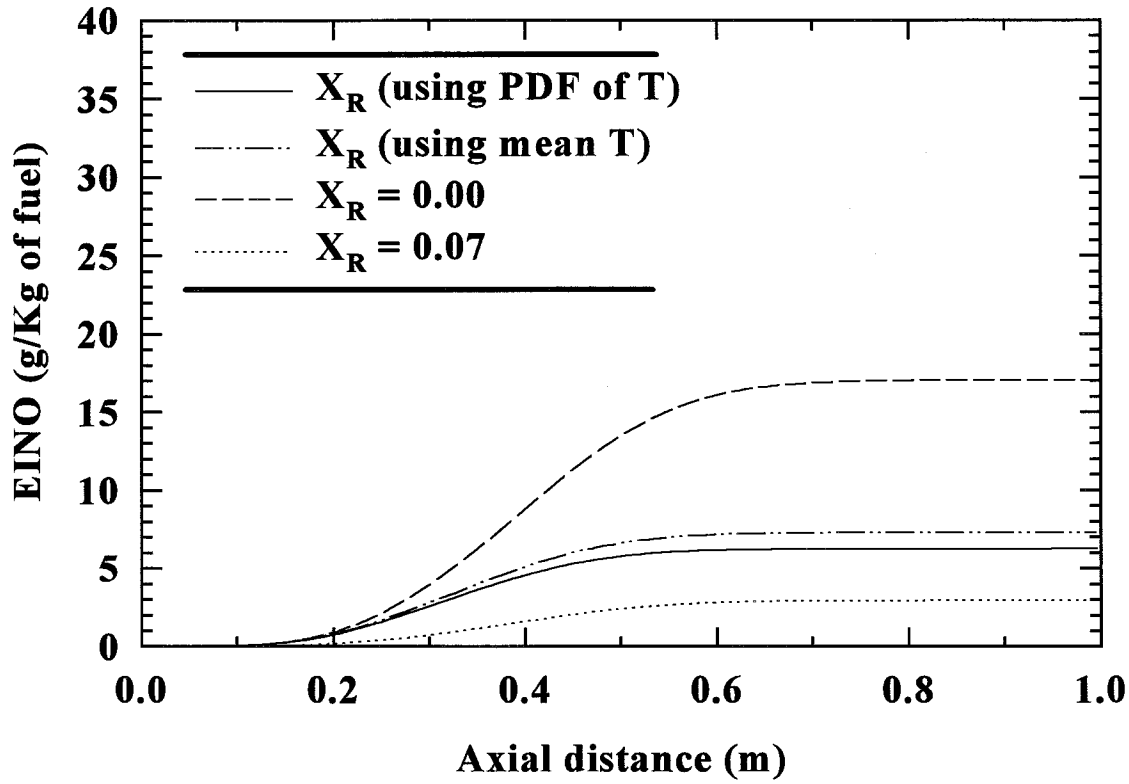

**State relationships for Hydrogen/air diffusion flame.**




**Predictions and measurements of radiative flux.**




**Predictions and measurements of radiative flux.**




**NO production as a function of axial distance.**

# CONCLUSIONS

- **Radiation measurements with emphasis on band structure of $H_2O$ are needed**
- **Optically thin assumption** $\rightarrow \int_o^{\Delta s} a_\lambda \, ds << 1$
- **Emission approximation** $\rightarrow \Pi_{ae} = \dfrac{a_i \Pi \bar{i}_i}{a p_{ch} \sigma T_{ch}^4} << 1$
- **For $H_2$/air flames maximum** $\Pi_{ae} \sim 0.2$
- **State relationships for $N_2$ and $O_2$ based on experimental laminar flamelet state relations do not yield good NO predictions.**