Comparative study of transported scalar PDF and velocity-scalar PDF approaches to Delft Flame III

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Presented at "CFD in CRE IV", Barga, Italy, June 19-24, 2005

Outline

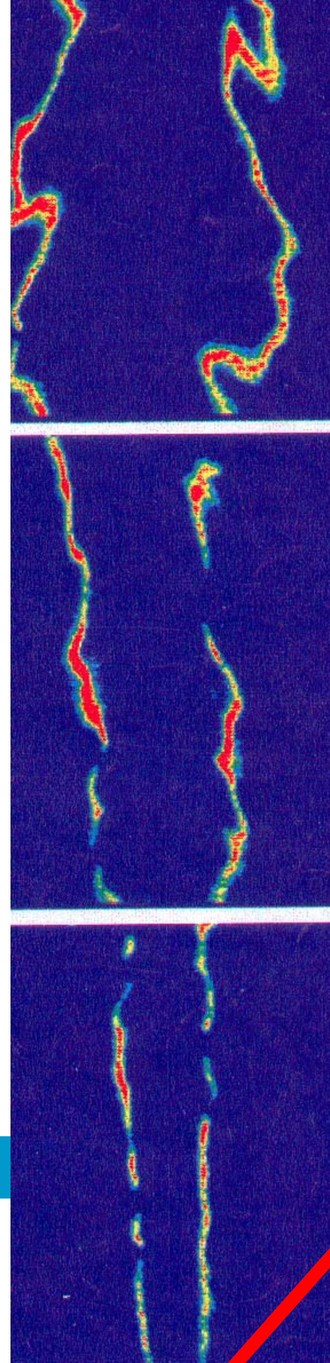
- Delft Flame III
- PDF methods
- Comparison velocity-scalar PDF vs scalar PDF results
- Sensitivity analysis of scalar PDF results
  (role of micromixing model, kinetic model …)
- Conclusions

Piloted natural-gas / air jet diffusion flame

PLIF of OH-radical showing:

- Instantaneous flame front position

- Local extinction



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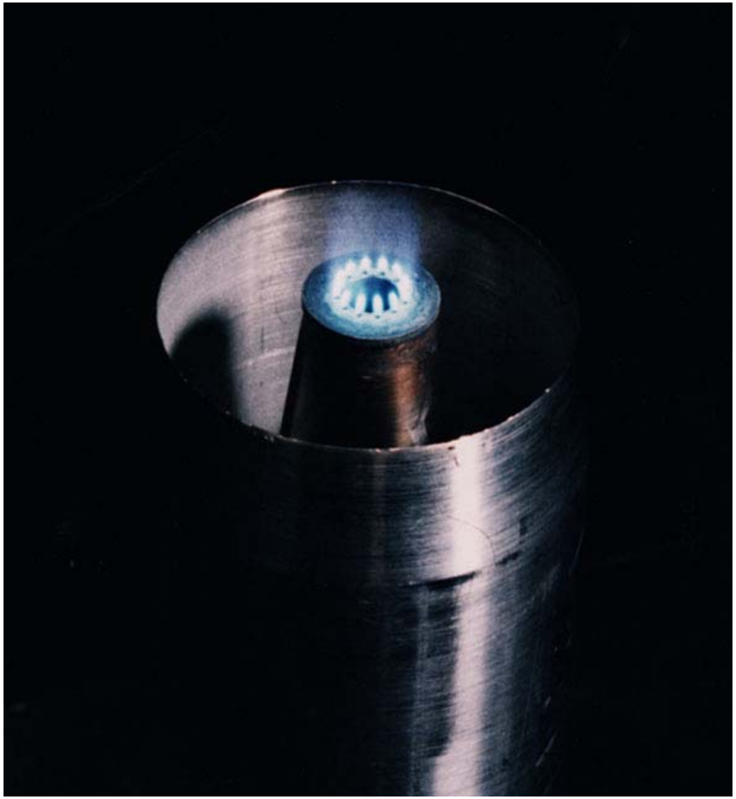
Closer view of the burner exit with burning pilot flames

- **Burner dimensions:**

Central fuel jet	radius = 3 mm
Rim	from 3 mm to 7.5 mm
Annular air jet	from 7.5 mm to 22.5 mm

- **Pilot geometry:**
12 nozzles of 0.5 mm
on a circle of 7mm diameter

- **Pilot fuel composition:**
mixture of C2H2, H2, air with - equivalence ratio 1.4
- same C/H ratio as main fuel
- thermal power 1 % of power of main flame



Experimental data base for Delft flame III

- Velocity (LDA)
- Main species and temperature (Raman-Rayleigh)
- Temperature (CARS)
- Minor species (OH-PLIF)

RANS modeling faces unclosed terms

Mean velocity	Reynolds Stress	Pressure-Strain correlation Triple correlation
Mean scalar	Reynolds flux	Pressure scrambling Triple correlation Velocity-Source correlation
	Mean Source	

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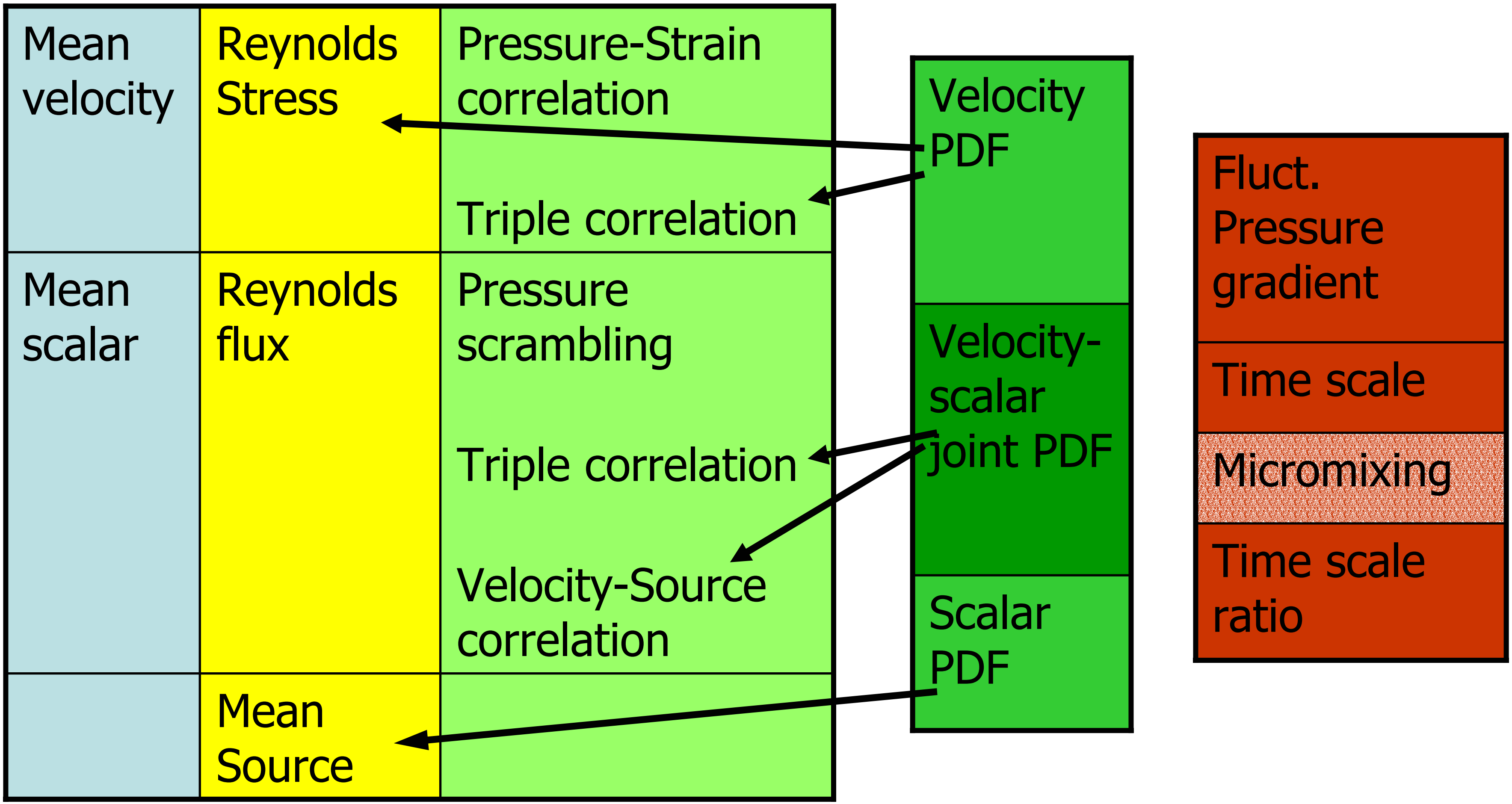
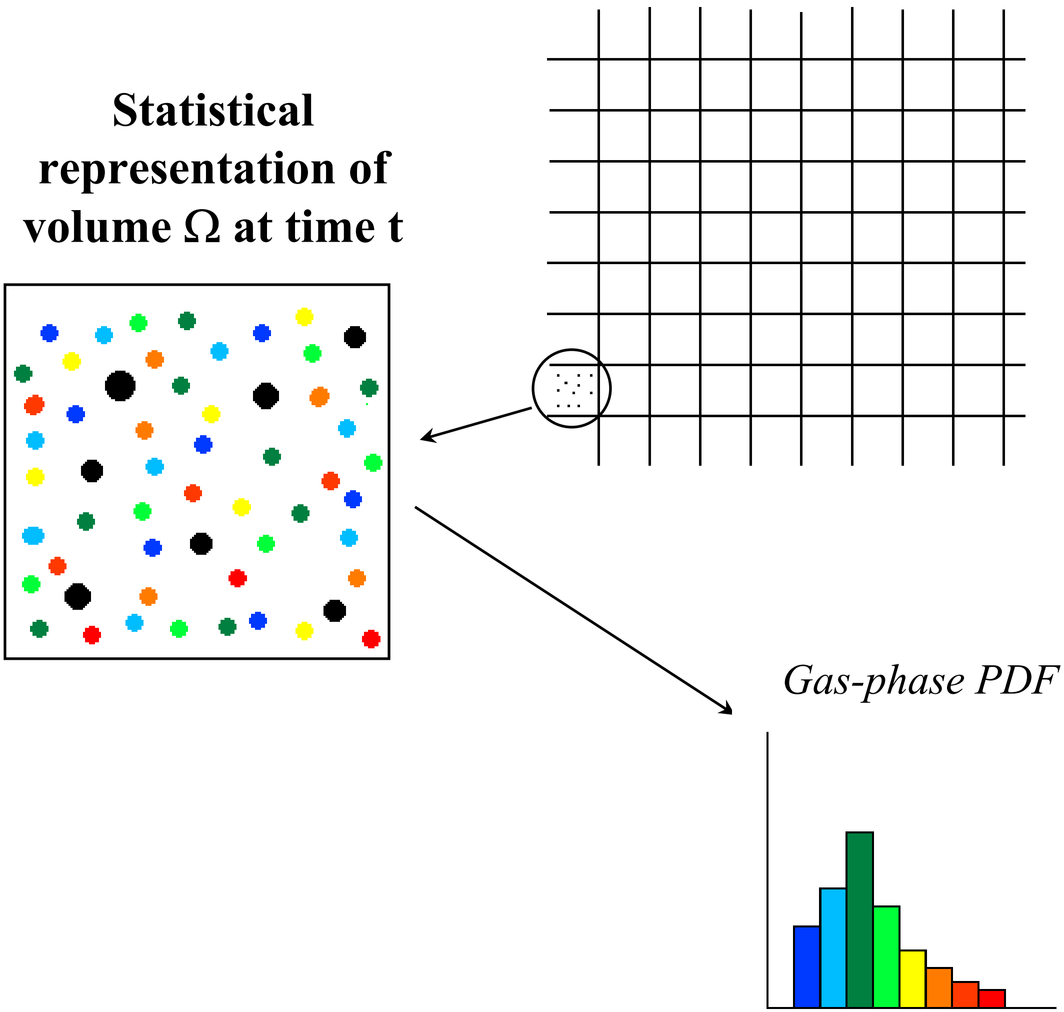
PDF modeling solves/faces closure problem



Representation of the gas phase PDF



Submodels

- Motion in space
- Micro-mixing
  - **IEM** (Interaction by Exchange with the Mean)
  - **CD** (modified Curl's Coalescence/Dispersion)
  - **EMST** (Euclidean Minimum Spanning Tree)
- **Chemistry**
  - Intrinsic Low Dimensional Manifold (**ILDM**)
    1 non-reacting and 2 reacting scalars
  - Skeletal scheme of **Correa** (16 species, 41 elementary reactions)
  - Skeletal scheme of **Smooke** et al. (16 species, 31 elementary reactions)
  - ARM (Augmented Reduced Mechanism): 9 species, 5 global reaction steps (derived from GRI2.11, ref. **Mallampali**)

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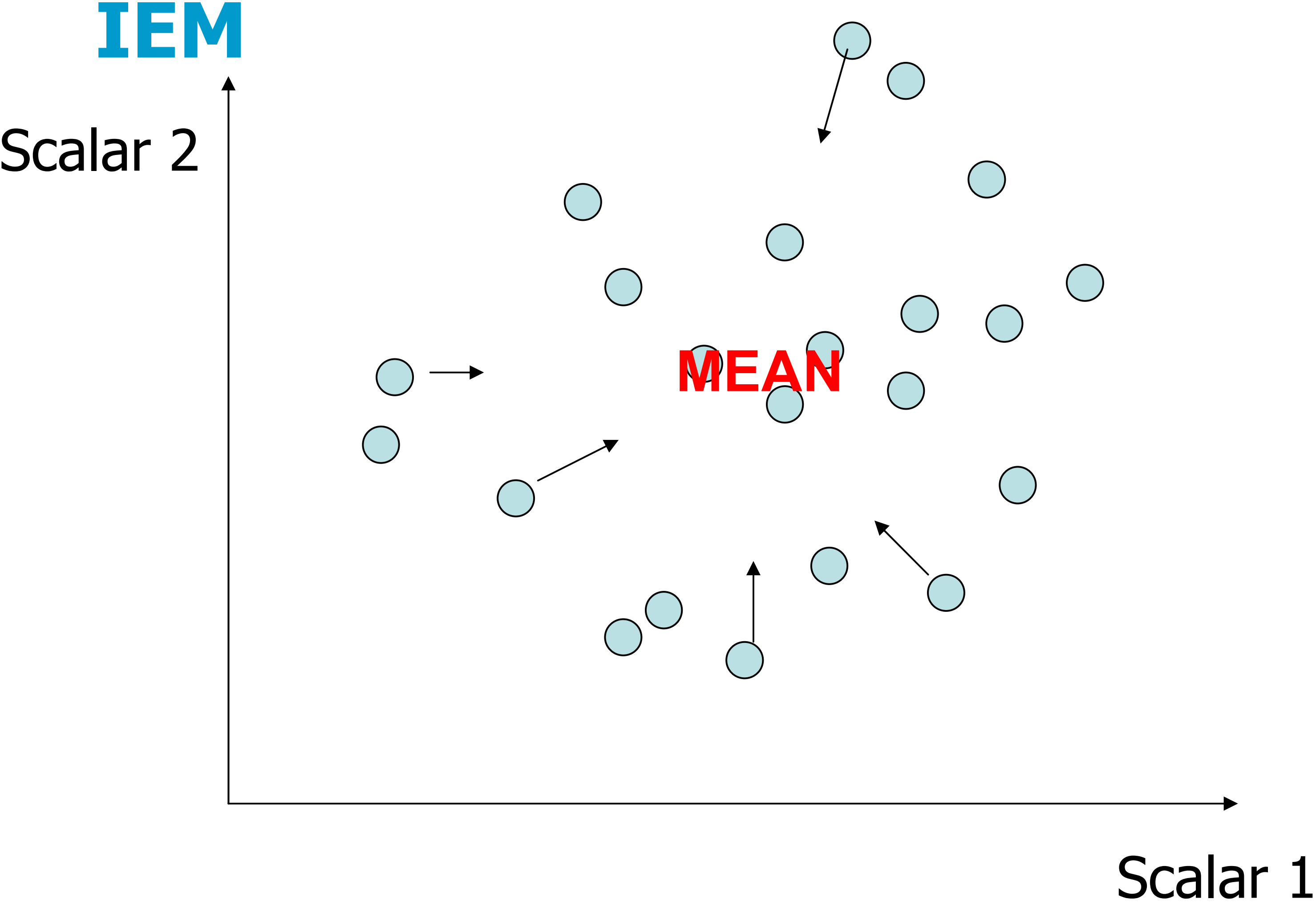
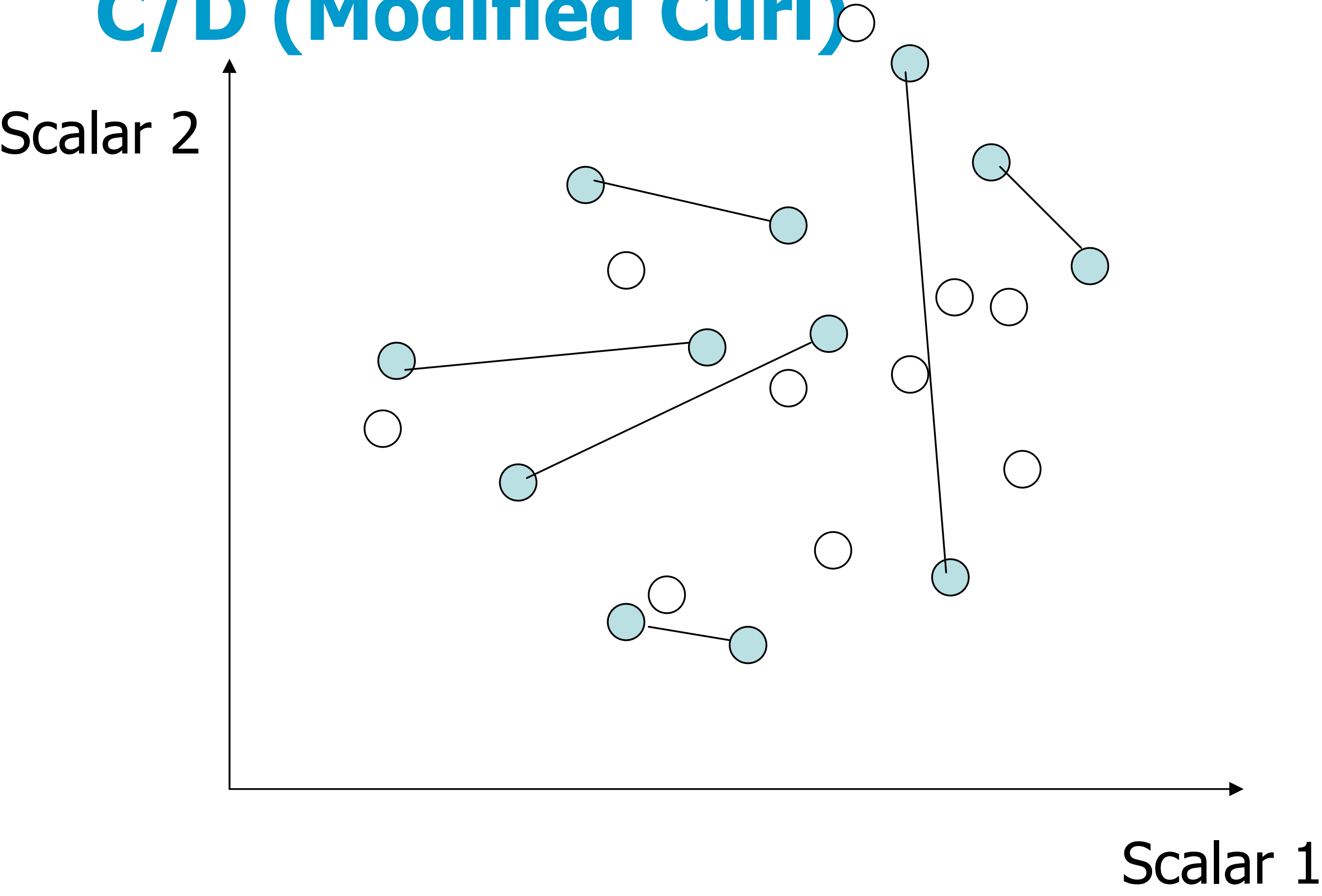
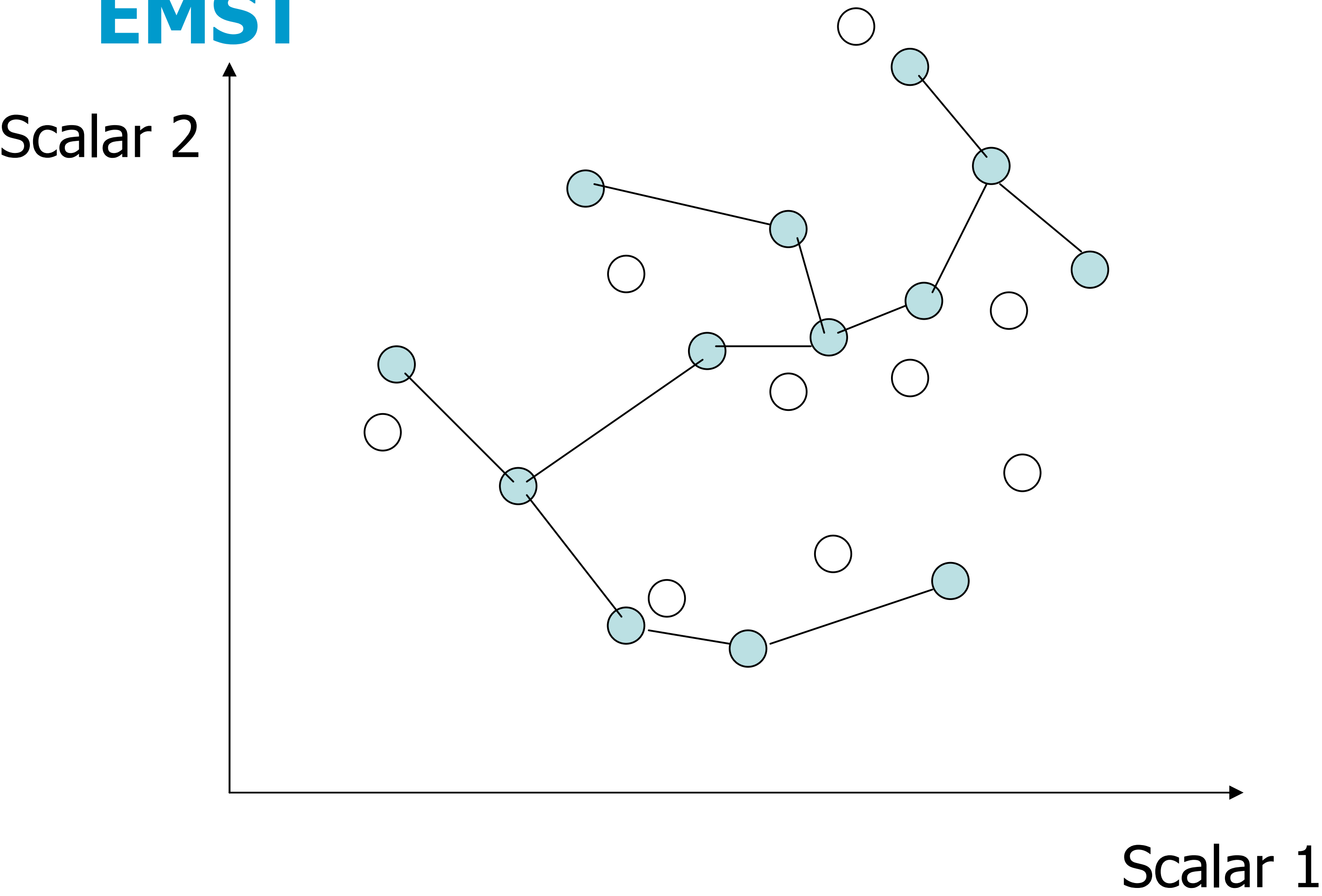
IEM



C/D (Modified Curl)



EMST



EMST:
Euclidean Minimal Spanning Tree

- Essential feature: mixing is modeled locally in composition space
- The particles are divided in two groups, participating and non-participating in mixing events. Particles change group after a randomly chosen time related to turbulent mixing time.
- The EMST for the compositions of the mixing particles is determined.
- The particles mix with neighbours in the EMST.

http://mae.cornell.edu/~laniu/emst.

PDF calculations of Delft flame III using finite rate chemistry

	Velocity	Micromixing	Chemistry
P.A. Nooren et al.	k-ε+round jet corr. Velocity scalar PDF	C/D	ILDM (dim=3)
B. Merci et al.	Nonlinear k-ε Scalar PDF	IEM, C/D, EMST	C1-chemistry with ISAT
		C/D, EMST	3 different kinetic schemes

Velocity-scalar PDF : TU Delft code
Scalar PDF: Fluent 6.2

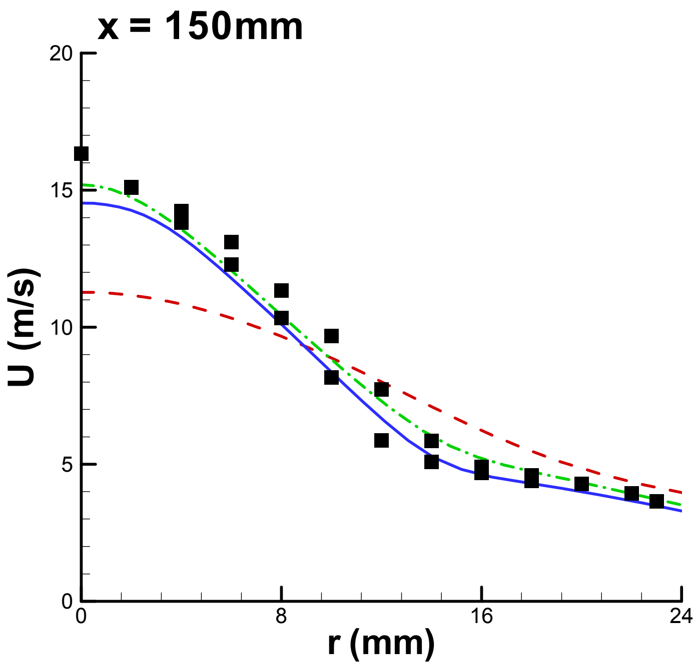
C1-chemistry: 16 species, 41 reactions

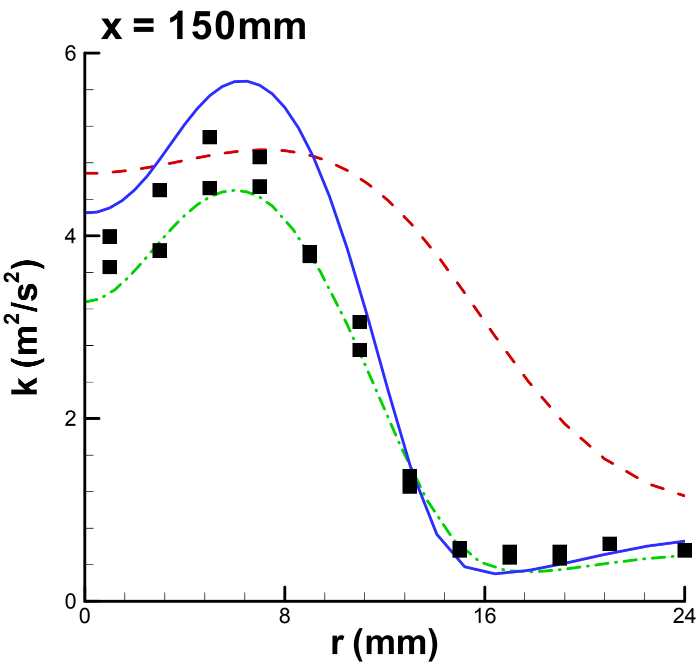
Radial profiles of mean axial velocity and turbulent kinetic energy

Standard k-ε

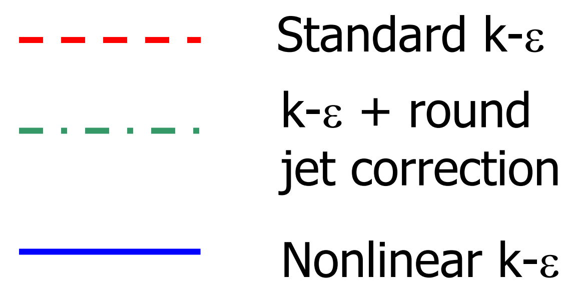
k-ε + round jet correction

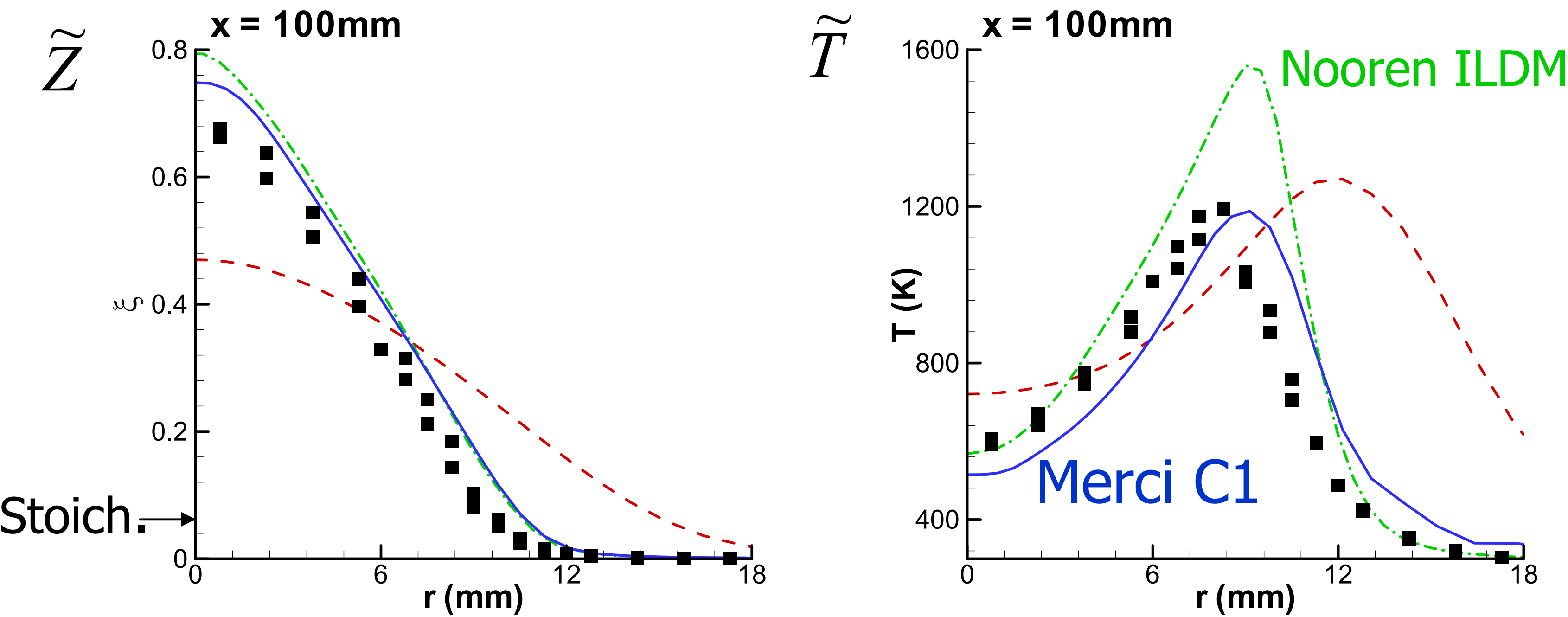
Nonlinear k-ε





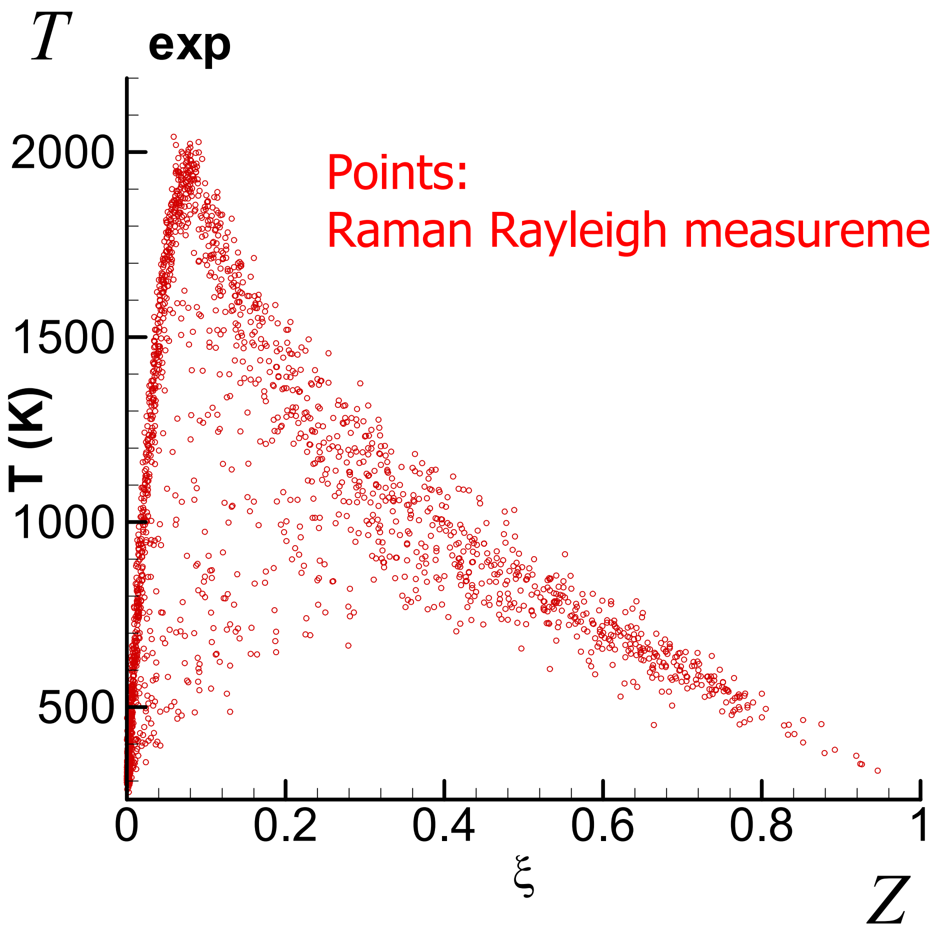
Radial profiles of mean mixture fraction and mean temperature





C/D micromixing used in all cases

Joint PDF of temperature and mixture fraction



At x =100 mm

Experimental results by P.A. Nooren et al.

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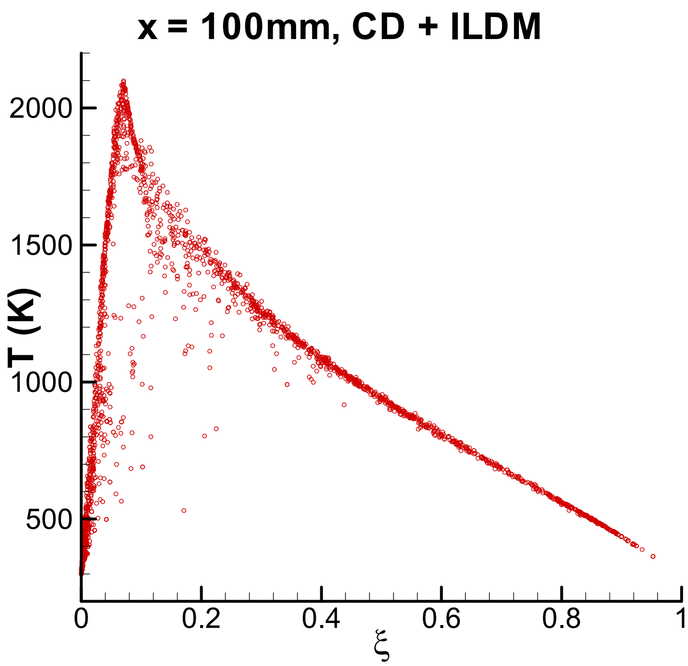
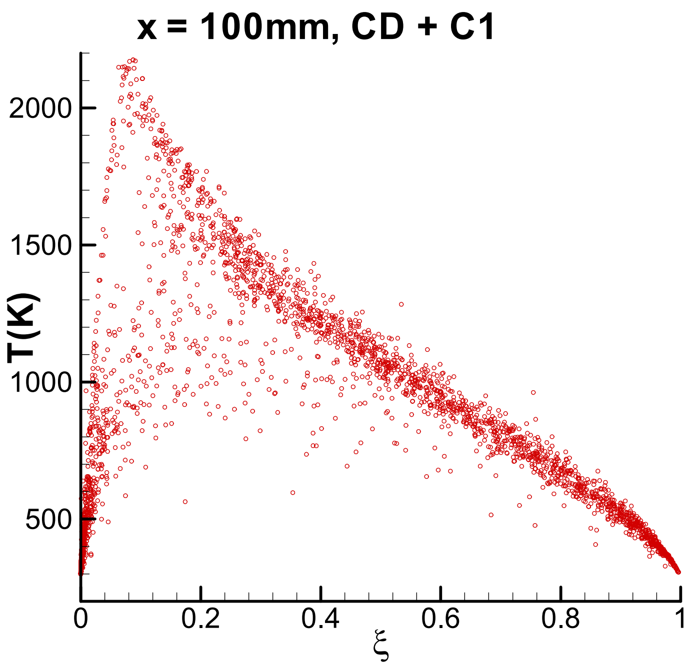
Joint PDF of temperature and mixture fraction

Computational results



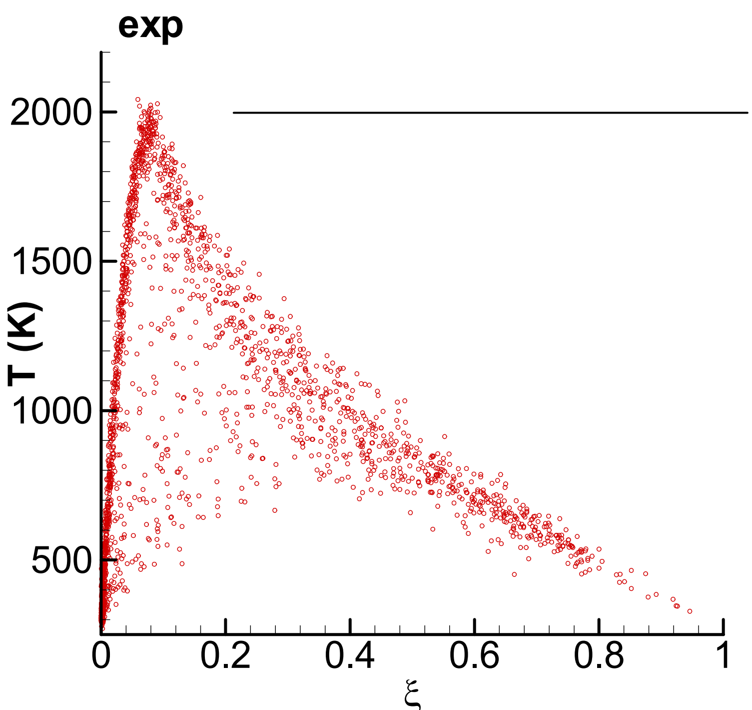
Nooren ILDM



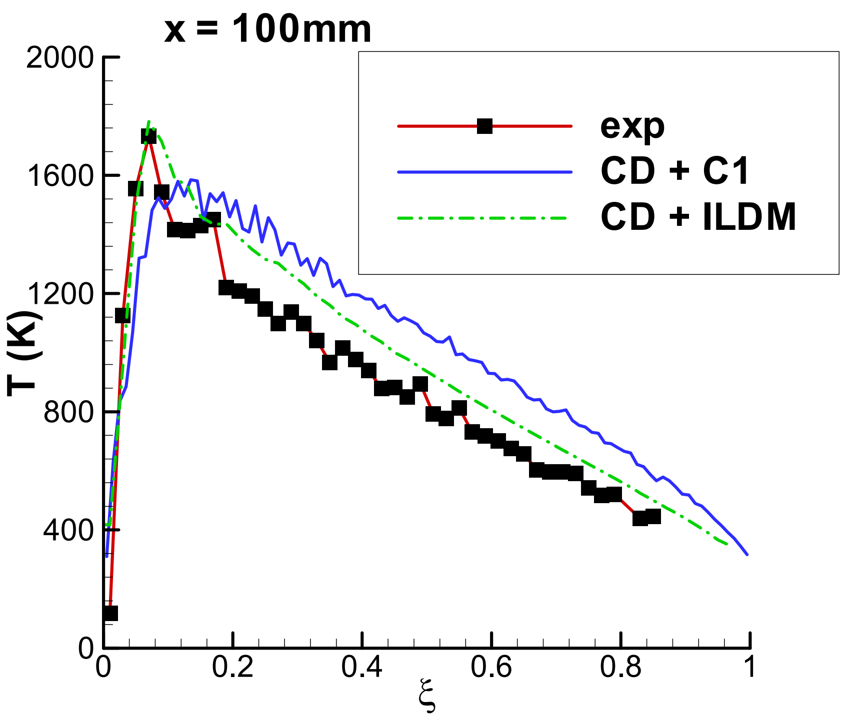
Merci C1

C/D micromixing used in both cases

Joint PDF of temperature and mixture fraction →Conditional mean temperature



Points:
RR measurements



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Conclusions part 1

Difference between velocity-scalar PDF results (Nooren) and scalar PDF results (Merci) mainly due to:

-Difference in chemistry model (ILDM vs C1-scheme)

-Difference in representation of the pilot flame (as flame or as heat source)

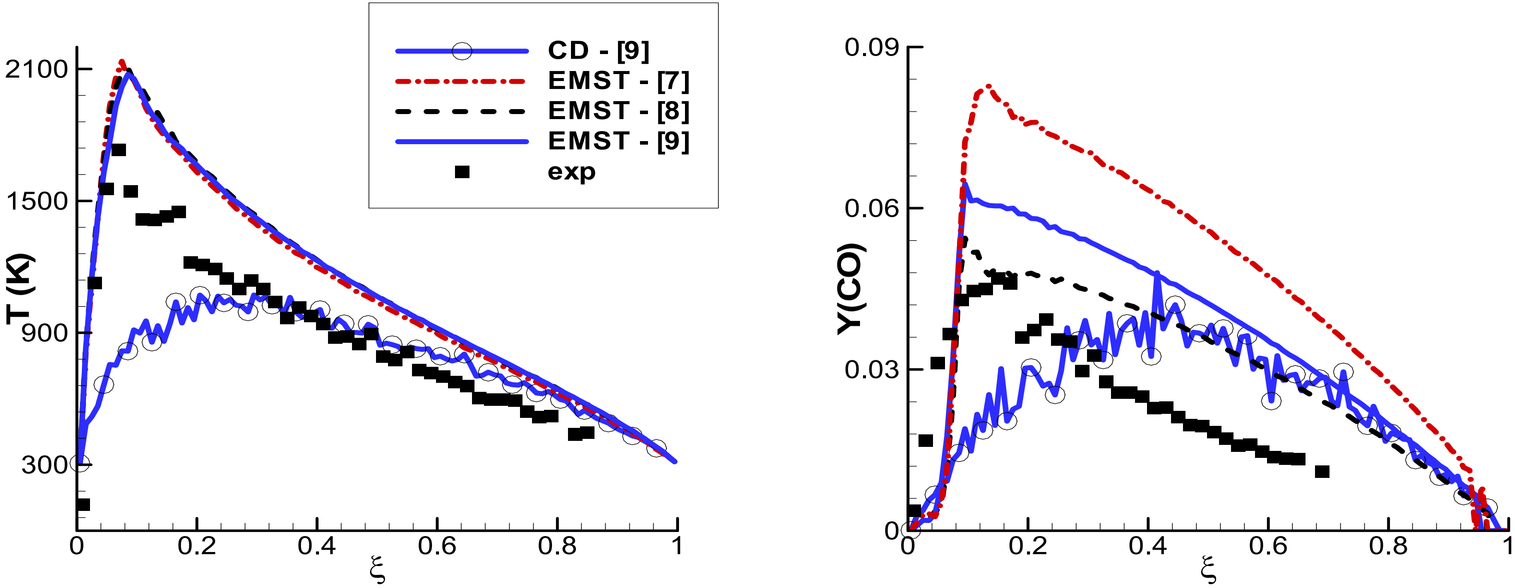
Sensitivity analysis scalar PDF results

Micromixing	Cphi	Kinetics	Pilot power (W)	Type of Flame
CD	2	Correa	200	Lifted
CD	3	Correa	200	Attached
CD	2	Correa	300	Attached
CD	2	Smooke	200	Attached
CD	2	Mallampali	200	Error …

Sensitivity results scalar PDF results

Micromixing	Cphi	Kinetics	Pilot power (W)	Type of Flame
EMST	2	Correa	200	Attached
EMST	2	Smooke	200	Attached
EMST	2	Mallampalli	200	Attached

EMST:
Influence of choice of kinetic scheme on CO conditional profile



Conclusions

Need better than standard k-eps to get flow field right

Need detailed chemistry to get local extinction right

Flame type:
IEM predicts blow off
CD predicts lifted or attached flame depending on details
EMST predicts attached flame

Next steps:
- use information from 3D simulation of pilot flames
- improve CD micromixing model

References

- Bart Merci, Bertrand Naud and Dirk Roekaerts,
  Flow and Mixing Fields for Transported Scalar PDF Simulations of a Piloted Jet Diffusion Flame ('Delft Flame III'), *Flow, Turbulence and Combustion*, in press

- Bart Merci, Dirk Roekaerts and Bertrand Naud,
  Study of the Performance of Three Micro-Mixing Models in Transported Scalar PDF Simulations of a Piloted Jet Diffusion Flame ('Delft Flame III'), *Combustion and Flame*, in press

- B. Merci, B. Naud and D. Roekaerts,
  Interaction between chemistry and micro-mixing modeling in transported PDF simulations of turbulent non-premixed flames,
  Mediterranean Combustion Symposium, Lisbon, October 6-10, 2005

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