Implementation of Combustion Models for Large-Eddy Simulation

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Introduction

- LES of combustion problems in OpenFOAM: Weller b-Ξ model is currently the only choice
- Extension of model selection desirable
- Current work:
  - Implementation and verification of artificially thickened flame model and presumed-PDF model (mainly for premixed/partially premixed combustion)

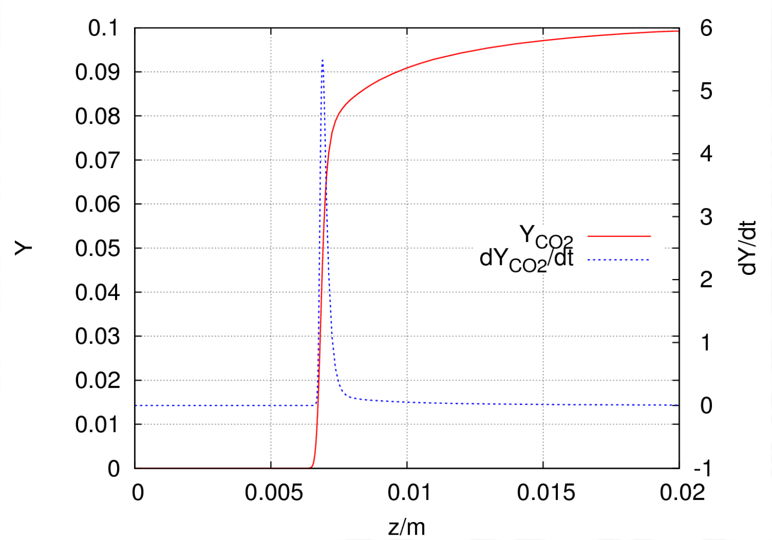
Presumed-PDF

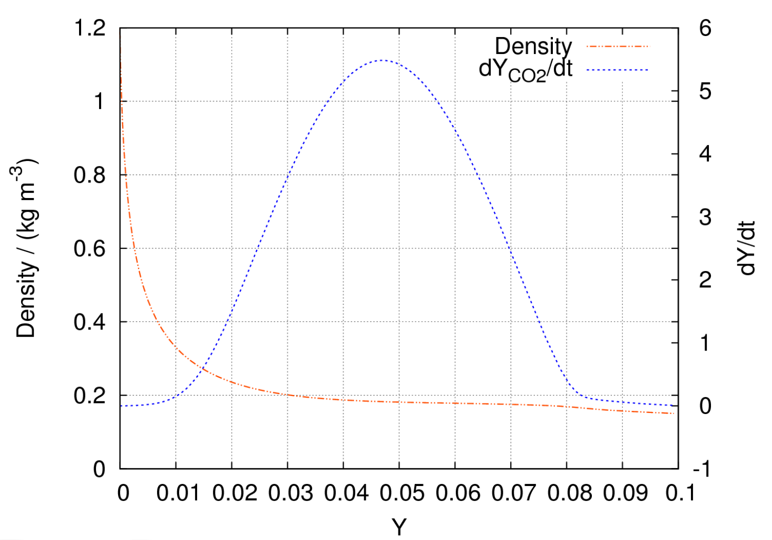
- Three stages:
  1. Tabulation of mixture properties and source terms as functions of controlling variables
  2. Integration over PDF's
  3. Solver:
     - Transport equations for
       - mean and
       - variance of controlling variables
     - Lookup of mean source terms and mixture properties

Preprocessing

1. Generation of Chemistry-Tables

- Currently implemented: Flamelet-Generated Manifolds (FGM)
  - Laminar flamelet is interpreted as 1D low-dimensional attracting manifold in chemical state space





CANTERA is used for laminar flame computations

2. Presumed-PDF Integration

- PDF-Integration is Preprocessing-Step

$Y_1, Y_2, \dots$	$T, \rho, c_p, \dot{\omega}_1, \dot{\omega}_2, \dots$
$\vdots$	$\vdots$

$\Rightarrow$ PDF

$\tilde{Y}_1, \widetilde{Y'^2}_1, \tilde{Y}_2, \widetilde{Y'^2}_2, \dots$	$\tilde{T}, \tilde{\rho}, \tilde{c}_p, \tilde{\dot{\omega}}_1, \tilde{\dot{\omega}}_2, \dots$
$\vdots$	$\vdots$

  - Lookup-Table class can handle structured tables of arbitrary dimensionality

- PDFs are run-time selectable
  - beta-PDF
  - clipped gaussian
- Integration is done numerically
  - To circumvent singularities: PDFs are decomposed into sum of smooth distribution and weighted Dirac-deltas

$$P_1(x) = p_1(x) + \sum_{i=0}^{n_1} c_{1i}\,\delta(x - x_{\delta i}) \qquad P_2(y) = p_2(y) + \sum_{j=0}^{n_2} c_{2j}\,\delta(y - y_{\delta j})$$

2. Presumed-PDF Integration

- Multiplication of PDF's then splits integral:

$$\int_0^1 \int_0^1 f(x,y) P_1(x) P_2(y)\, dx\, dy = \int_0^1 \int_0^1 f(x,y) p_1(x) p_2(y)\, dx\, dy +$$

$$\sum_{j=0}^{n_2} c_{2j} \int_0^1 f(x, y_{\delta j})\, dx + \sum_{i=0}^{n_1} c_{1i} \int_0^1 f(x_{\delta i}, y)\, dy + \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} c_{1i} c_{2j} f(x_{\delta i}, y_{\delta j})$$

External numerical integration routines are used:

- For multidimensional integrals: CUBA library
  http://dx.doi.org/10.1016/j.cpc.2005.01.010
- For one-dimensional integrals: Gnu Scientific Library

Artificially Thickened Flame (ATF)

- Idea: artificially thicken the flame by factor F and leave flamespeed unchanged

$$s_l^0 \propto \sqrt{D\,\dot{\omega}} \qquad \delta_l^0 \propto \frac{D}{s_l^0}$$

Thickening by Factor F: $\bar{D} \leftarrow F\,D \qquad \bar{\dot{\omega}} \leftarrow \dot{\omega}/F$

$$\bar{s}_l^0 \propto \sqrt{F\,D\,\frac{\dot{\omega}}{F}} = s_l^0 \qquad \bar{\delta}_l^0 \propto \frac{F\,D}{s_l^0} = F\,\delta_l^0$$

- But: Turbulence-Flame interaction is altered, therefore flamespeed enhanced by efficiency factor E

Efficiency factor E: $\tilde{D} \leftarrow E\,\bar{D} \qquad \tilde{\dot{\omega}} \leftarrow E\,\bar{\dot{\omega}}$

$$\tilde{s}_l^0 \propto E\sqrt{F\,D\,\frac{\dot{\omega}}{F}} = E\,s_l^0 \qquad \bar{\delta}_l^0 \propto \frac{E\,F\,D}{E\,s_l^0} = F\,\delta_l^0$$

Implementation of ATF

- Solver is based on *hCombustionThermo* class with equations for
  - normalized fuel mass fraction **ft**
  - combustion regress variable **b**
- source term for **b** from one-step reaction scheme with fitted rate parameters

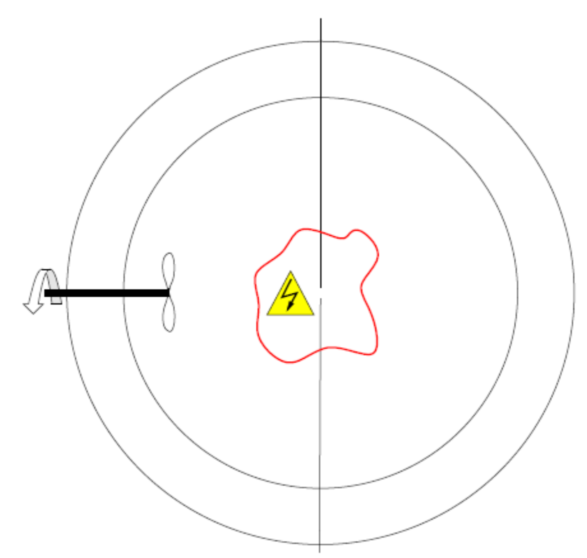
$$\dot{\omega}_b = -A[Fuel]^{\nu_F}[O_2]^{\nu_O}\exp\left(-\frac{T_a}{T}\right)$$

- Efficiency factor E from algebraic model according to *Colin* et al. (Phys. Fluids, Vol. 12(7) pp. 1843)

Testcases

- Turbulent Combustion Bomb
  - *Nwagwe* et al., Proc. Comb. Inst. Vol. 28, pp. 59
- Backward Facing Step
  - *Pitz & Daily*, AIAA J. Vol. 21(10) pp. 1565
- ORACLES
  - *Besson* et al., J. Thermophys. Heat Transfer Vol. 14, pp. 59
- Bunsen flame
  - *Chen* et al., Comb. and Flame Vol 107, pp. 223

Turbulent Combustion Bomb



Parameter	***Value***
Mixture	Propane/Air
Equivalence ratio	$\Phi=1$
Inital temperature	300K
Initial pressure	1bar
Velocity RMS	2.36m/s
Integral length scale	20mm

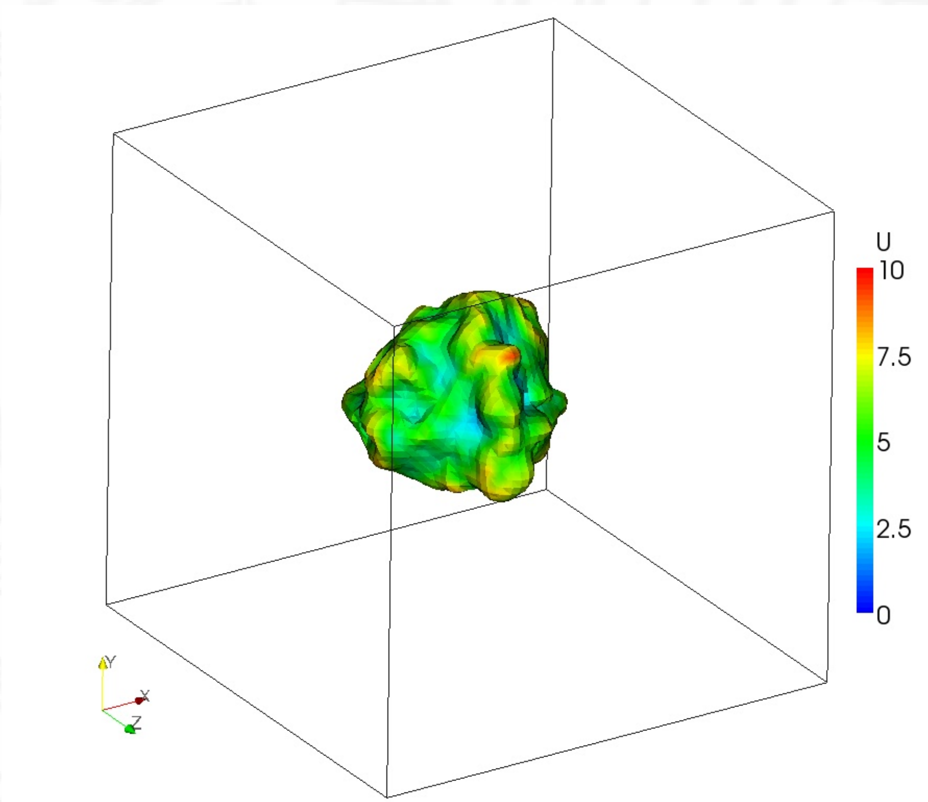
Characteristics

- Closed vessel
- Filled with premixed fuel/air
- Ignited in center by electric spark
- Turbulent initial velocity field by fan stirring

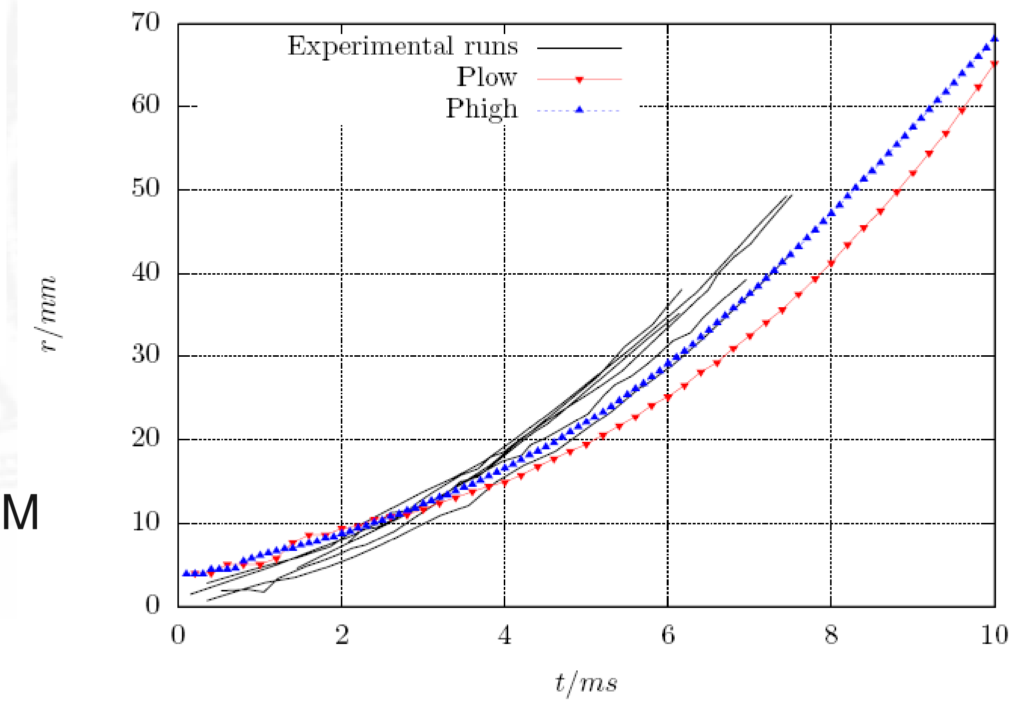
Numerical setup

- Simulation up to 3% of vessel volume to avoid pressure rise
- domain: cube with L=0.2m
- initial turbulent field by turbulent spot method (*Kornev* et al., Phys. Fluids Vol. 19(5))

Turbulent Combustion Bomb



Label	Combustion model	Remarks	Grid	Δ/δ_L^0
Plow	presumed-PDF		31^3	19.4
Phigh	presumed-PDF		64^3	9.4
Wlow1	Weller model	algebraic Ξ, unstrained s_L	31^3	19.4
Wlow2	Weller model	algebraic Ξ, equilibrium s_L	31^3	19.4
Wlow3	Weller model	transport Ξ, unstrained s_L	31^3	19.4
Whigh	Weller model	algebraic Ξ, unstrained s_L	64^3	9.4
TFlow1	Thickened Flame	$F = 20$	31^3	19.4
TFlow2	Thickened Flame	$F = 40$	31^3	19.4
TFhigh1	Thickened Flame	$F = 20$	64^3	9.4
TFhigh2	Thickened Flame	$F = 40$	64^3	9.4



Presumed-PDF/FGM
- beta-PDF

Turbulent Combustion Bomb

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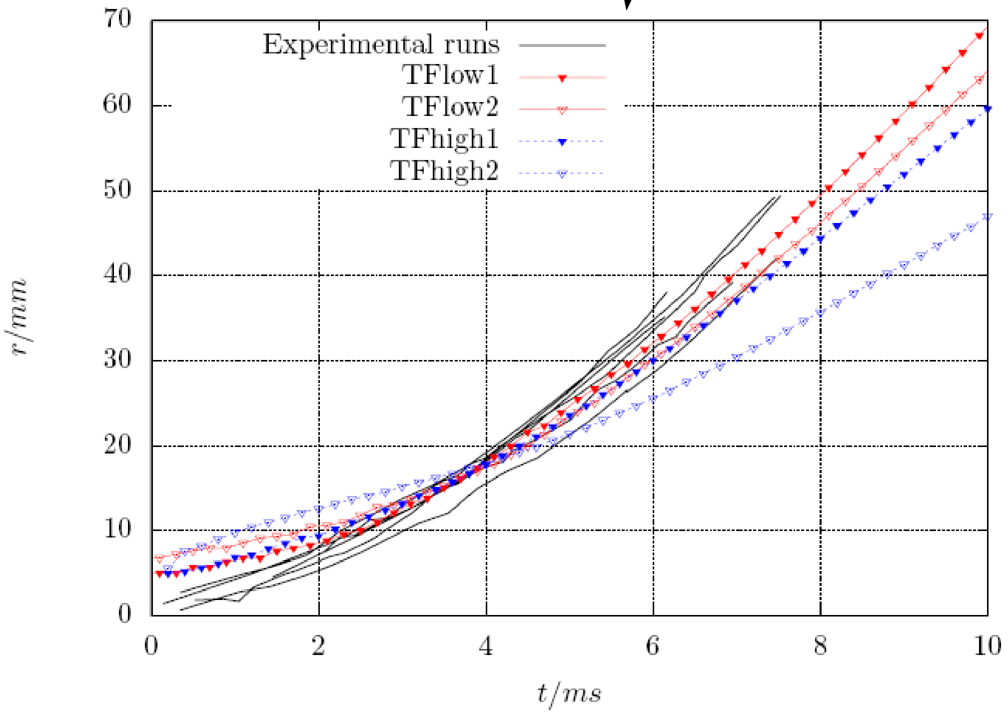
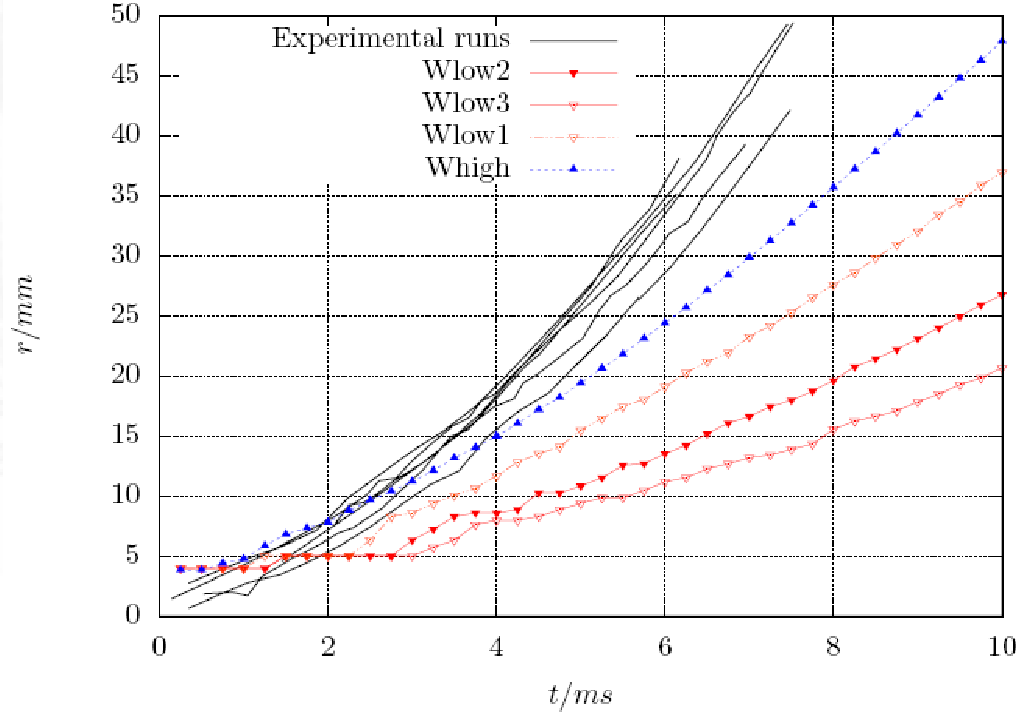
ATF model



Weller b-Ξ model



Backward-Facing Step

Propane/Air

Schlieren-
photograph

Characteristics

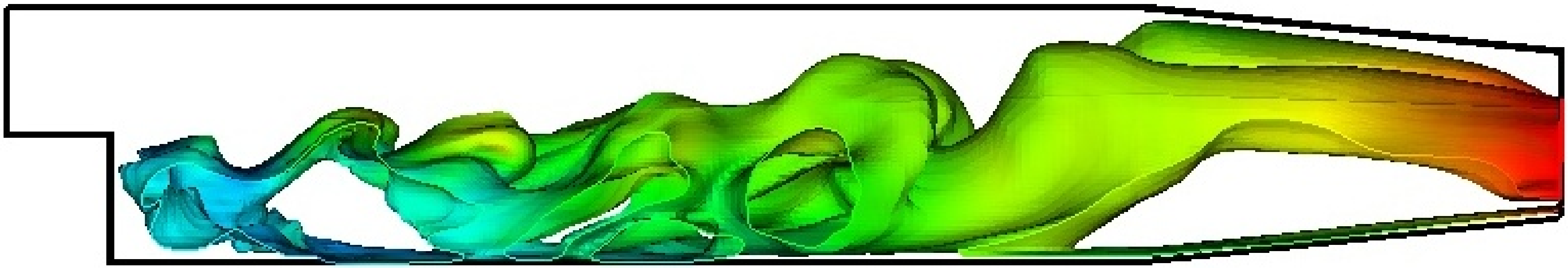
Cooled walls

$\Phi = 0.6$

$\bar{U} = 13.3\, m/s$

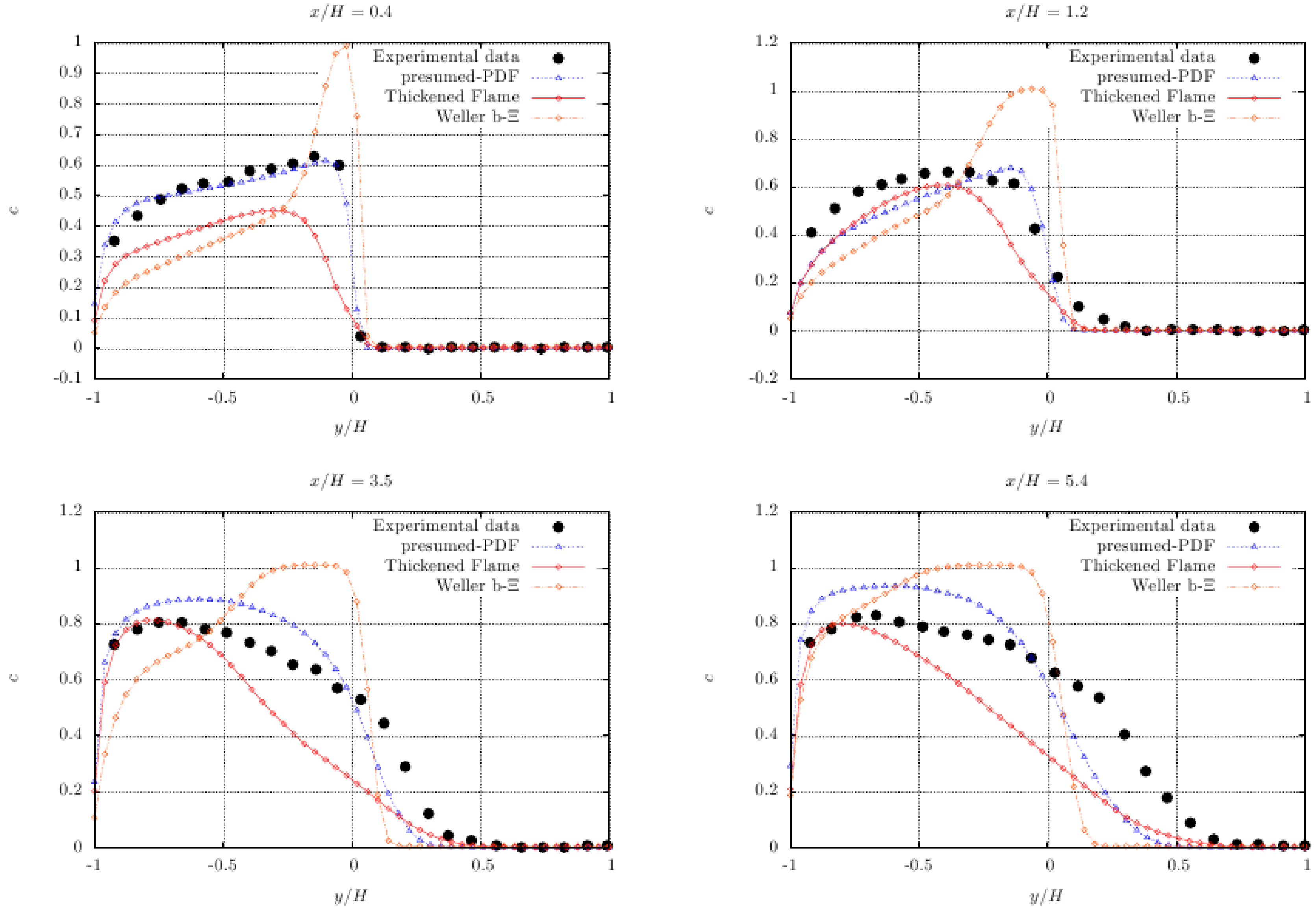
$\mathrm{Re} = 22100$

Presumed-
PDF

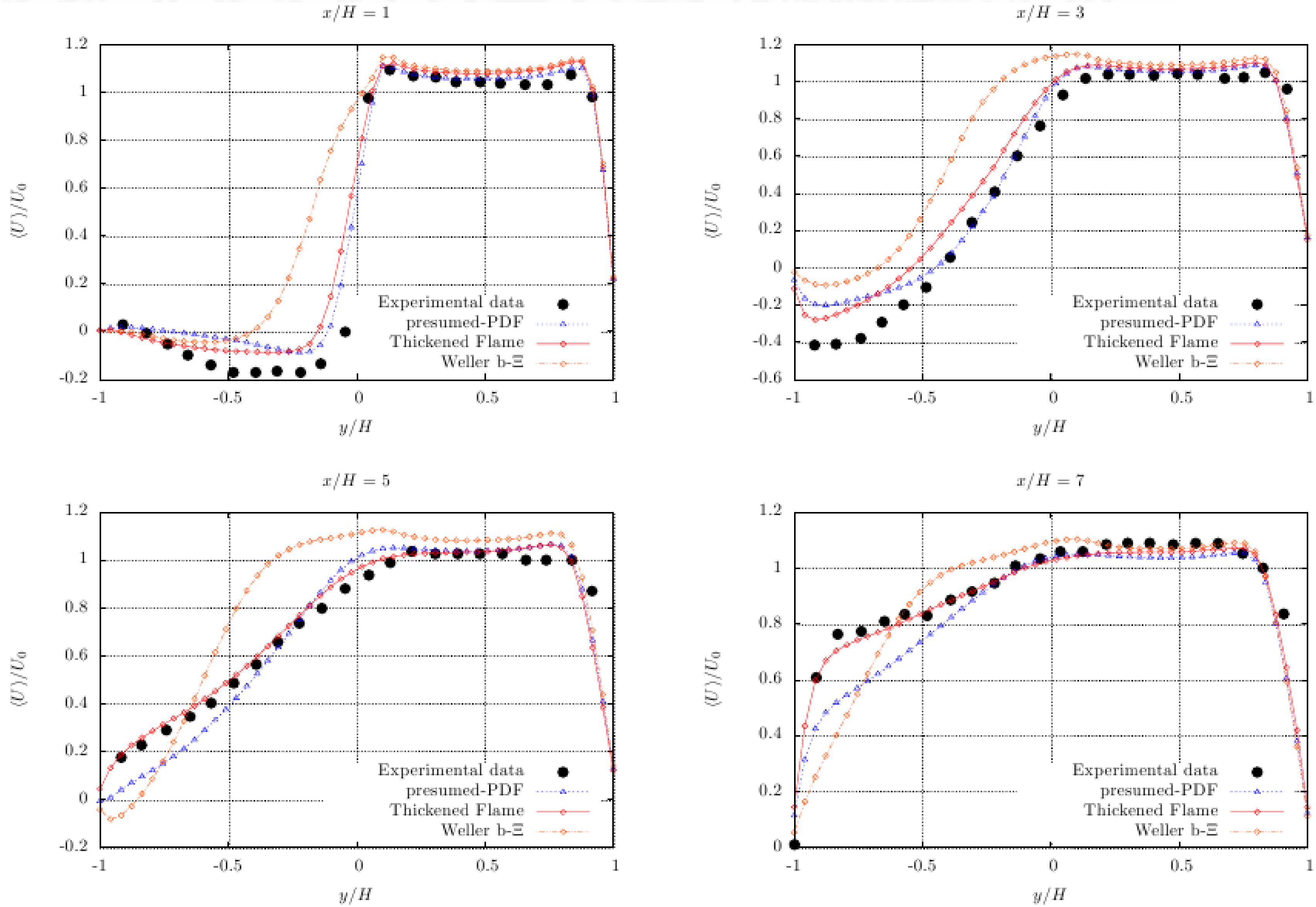


ATF

Backward-Facing Step: Mean Temp.

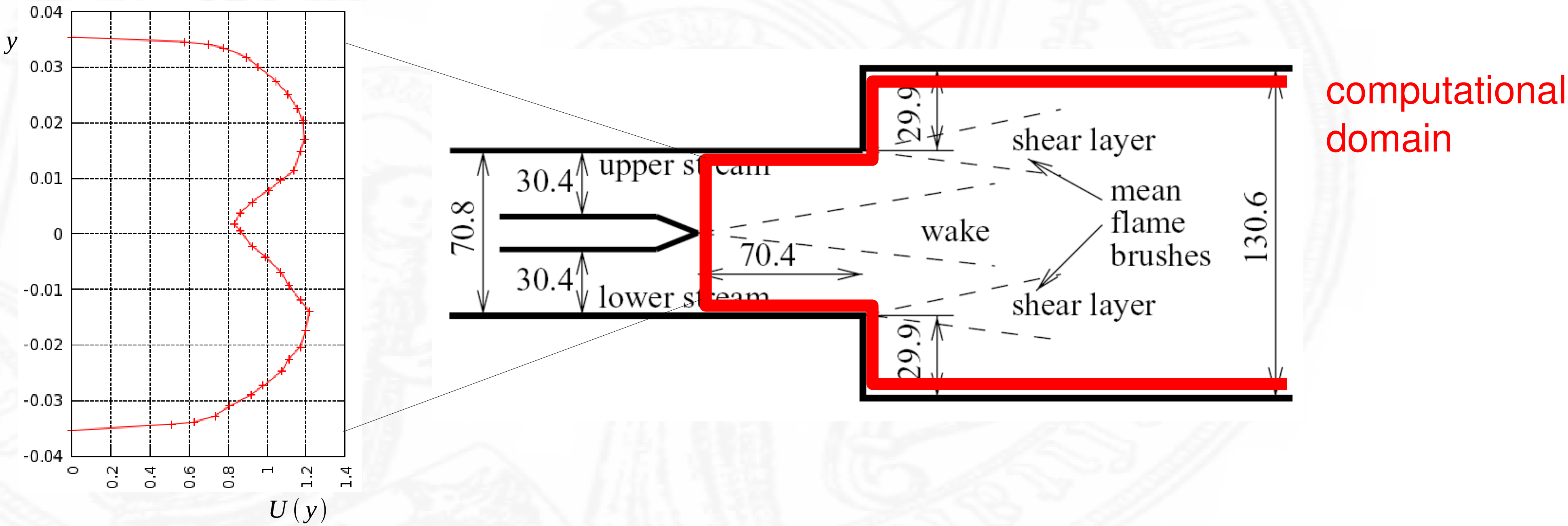


Backward-Facing Step: Mean Velocity



ORACLES

<u>O</u>ne <u>R</u>ig for <u>A</u>ccurate <u>C</u>omparison with <u>LES</u>

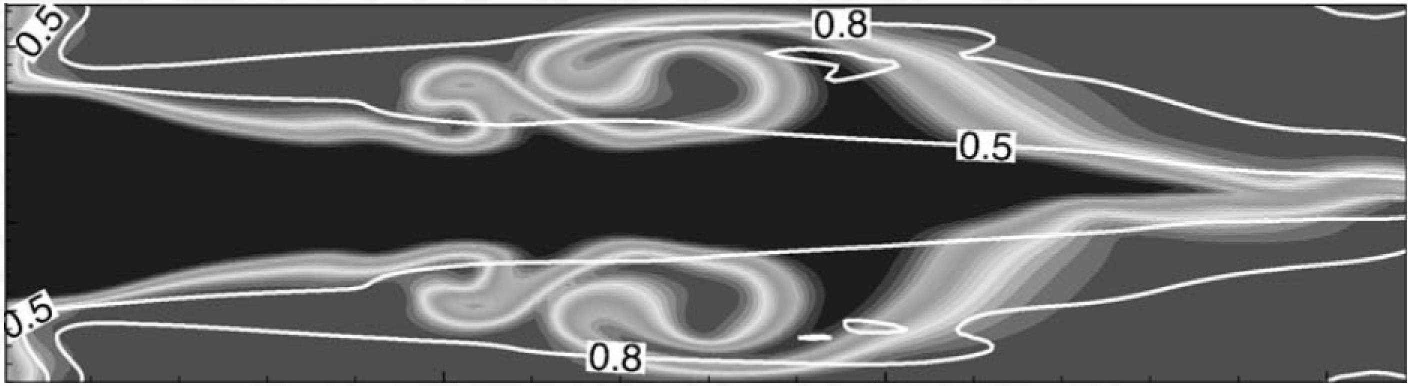


- Dominant acoustic oscillation occurs in feeding channels
- Sinusoidal forcing is applied to mimic acoustic mode (f=50Hz)

$$u(y,t)=U(y)[1+A\sin(2\pi f t)]+u'(y,t)$$

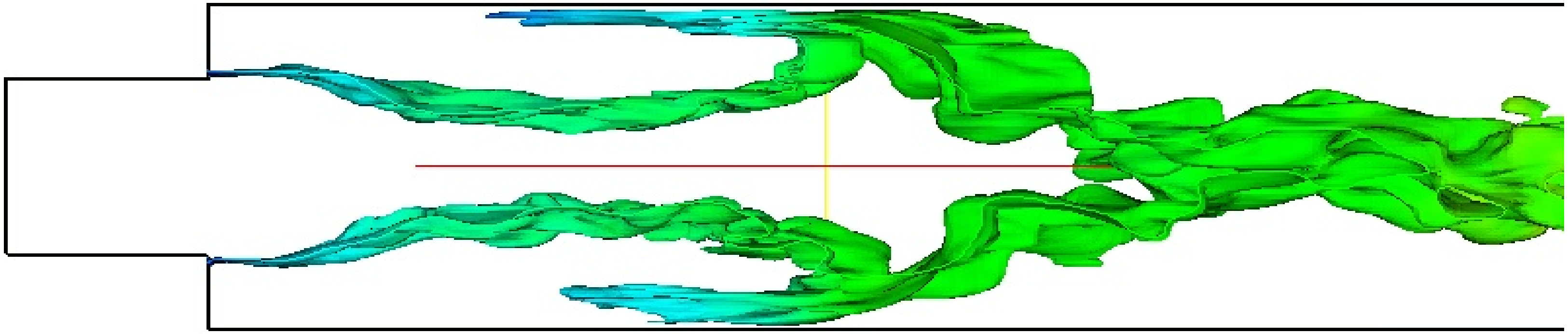
ORACLES

Contours of progress variable from Vervisch & Domingo



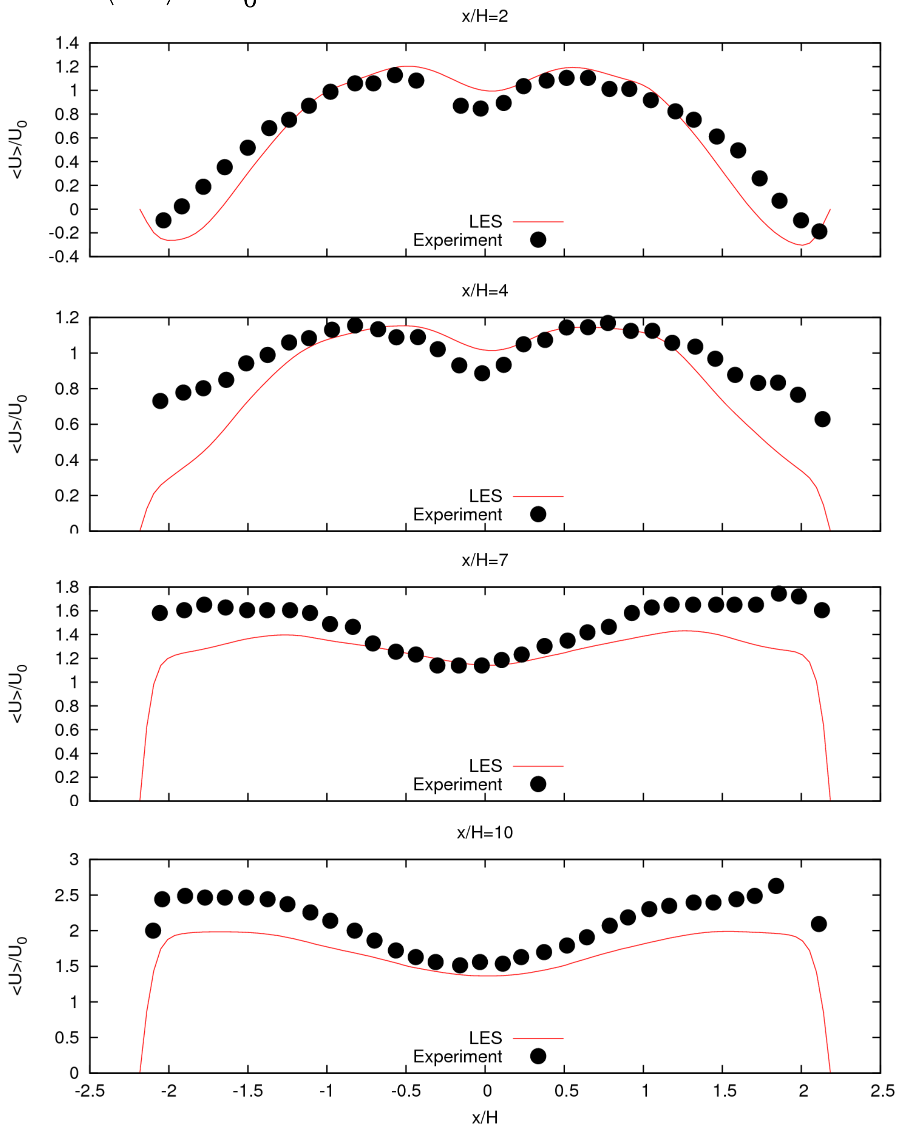
Ref.: Vervisch & Domingo, http://dx.doi.org/10.1016/j.crme.2006.07.008

Presumed-PDF model (Isosurface T=1000K)

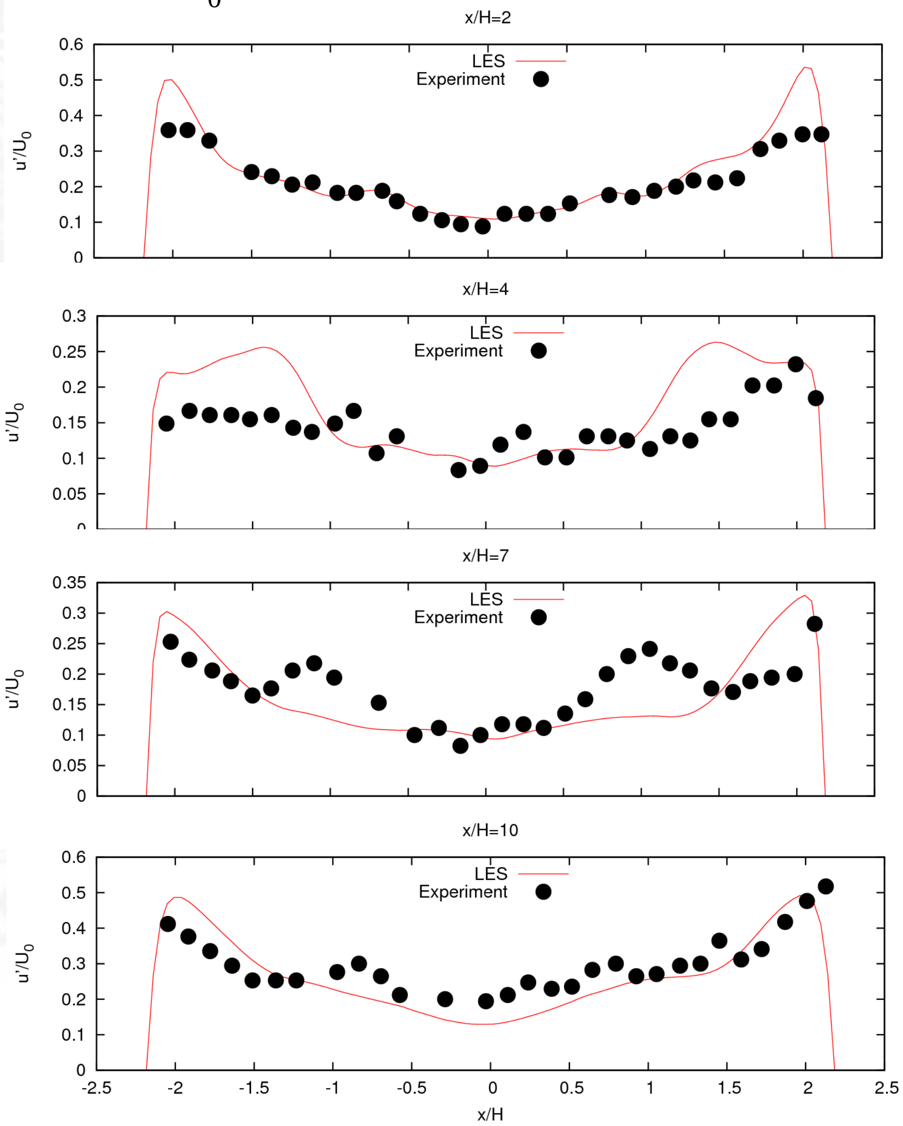


ORACLES: Mean Profiles

$\langle U \rangle / U_0$

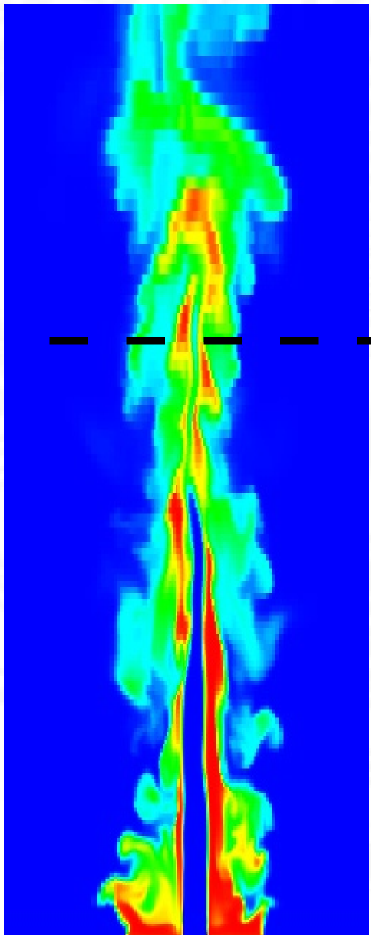


u' / U_0

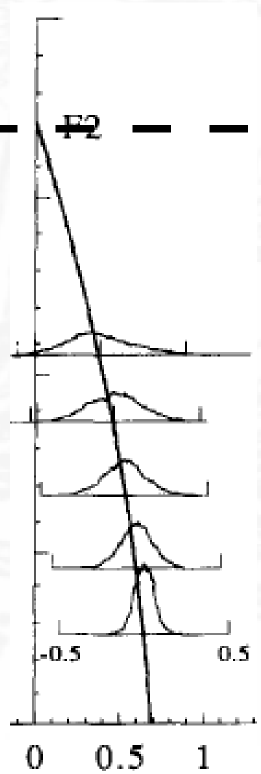


Bunsen flame F2

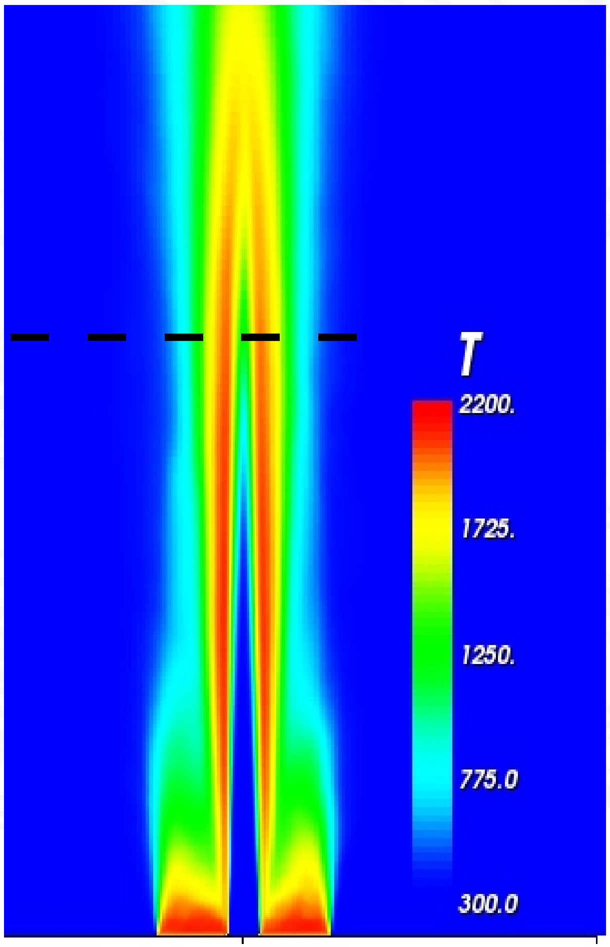
instantaneous temperature



exp. flame boundary

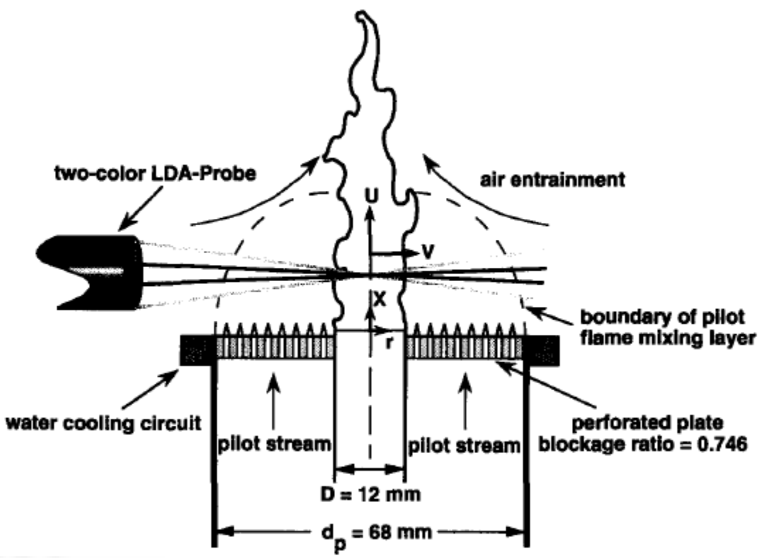


mean temperature



Characteristics

- partially premixed
- heat losses in coflow neglected
- inflow generator in nozzle

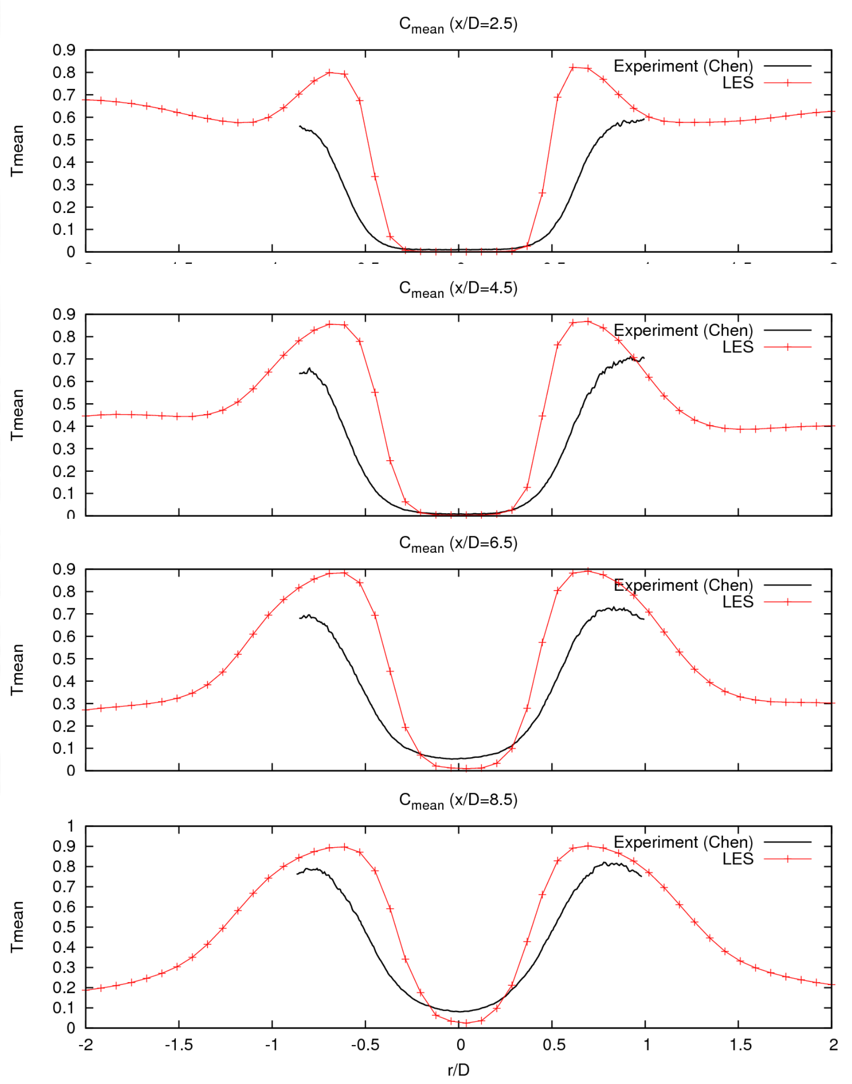


Global Flame Characteristics and Operating Conditions

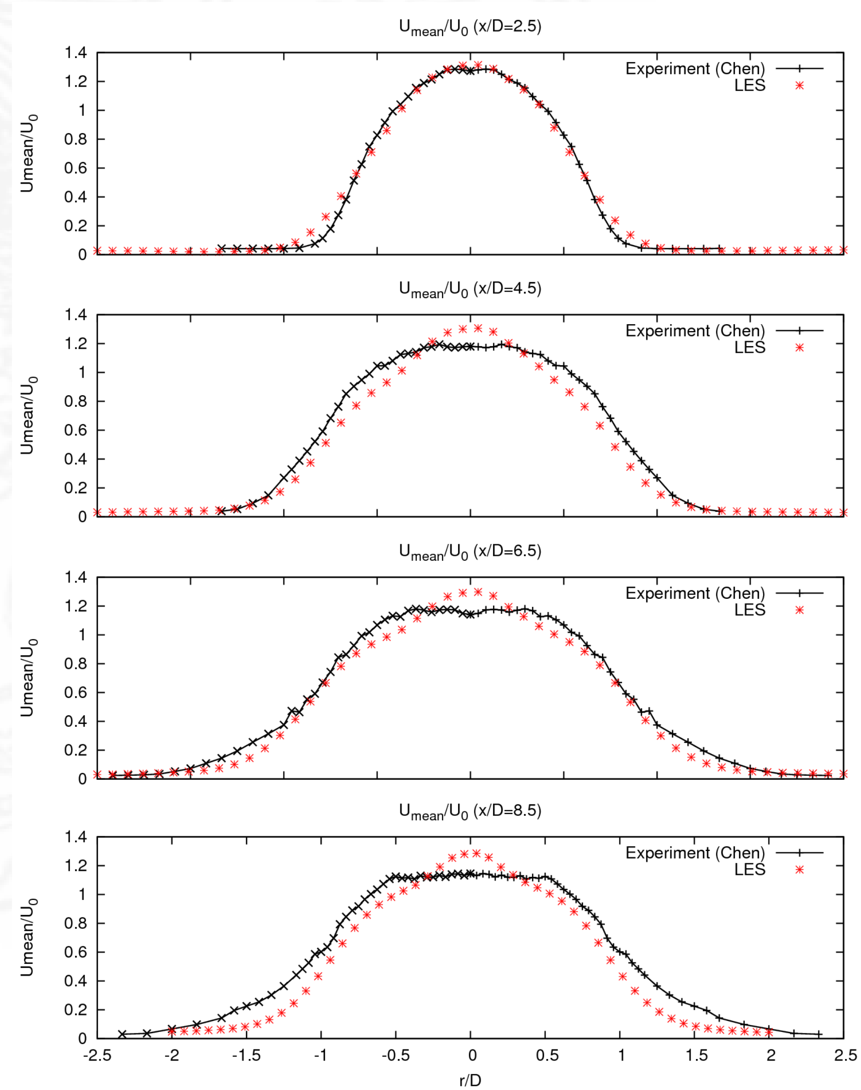
flame	F1	F2	F3
$U_0\ (m/s)$	65	50	30
H_i/D	37.5	33.3	27.5
H_c/D	12.5	10.5	8.5
L_i/D	2.83	3.75	5

Bunsen flame: Mean Profiles

$c=(T-T_u)/(T_{eq}-T_u)$



$\langle U \rangle / U_0$



Conclusions and Outlook

- Successful implementation of
  - presumed-PDF model and
  - artificially thickened flame model
- Simulations of testcases give encouraging results
- Source code available at LTT-Rostock SVN repository:

https://janus.fms.uni-rostock.de/svn/repository/OpenFOAM/trunk/LTTRostockExtensions

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