Imperial College London

Conference on Turbulence and Interactions
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Hydrogen autoignition using Eulerian Stochastic Fields method with LES

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Motivation

Autoignition

- Unsteady process
- Finite rate chemistry
- Turbulence–chemistry interaction

Autoignition Model Requirements

- LES or URANS
- ***No*** equilibrium, ***No*** fast chemistry approaches
- Models coupled with flow solver

Contents

- LES Combustion Model

  Sub-grid Probability density function (PDF)
- Eulerian Stochastic Fields method
- Results Hydrogen Autoignition
- Conclusions

LES Equations

Filtered variable

$$\bar{f} = \int_V G(\mathbf{x} - \mathbf{x}'; \Delta)\, f(\mathbf{x}')\, dx'$$

Favre filtering

$$\bar{\rho}\tilde{f} = \overline{\rho f}$$

Continuity

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0$$

Momentum

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{u}_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)\right] - \frac{\partial \tau_{sgs}}{\partial x_j}$$

Scalars (equal diffusivity)

$$\frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho}D\frac{\partial \tilde{Y}_k}{\partial x_j}\right] - \frac{\partial J^k_{sgs}}{\partial x_j} + \bar{\rho}\tilde{\omega}_k$$

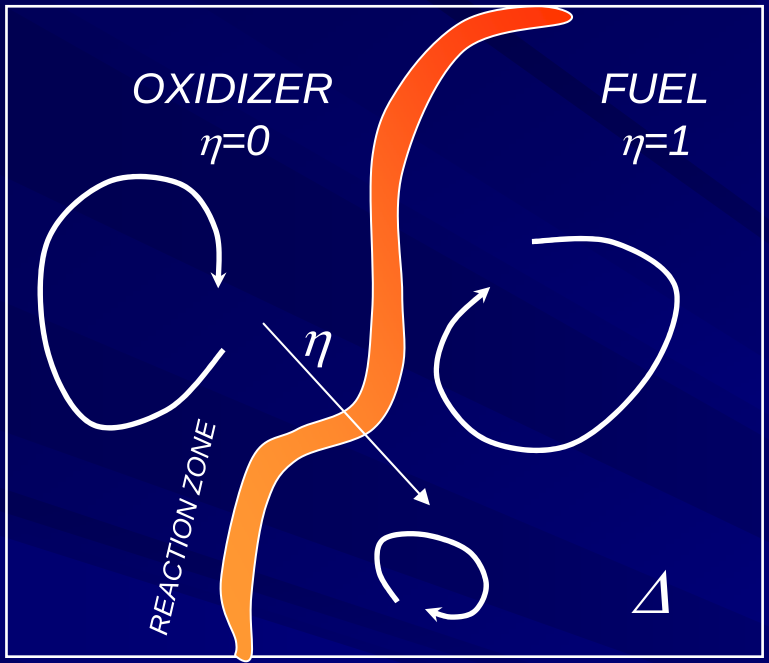
??? **Combustion SGS phenomena**

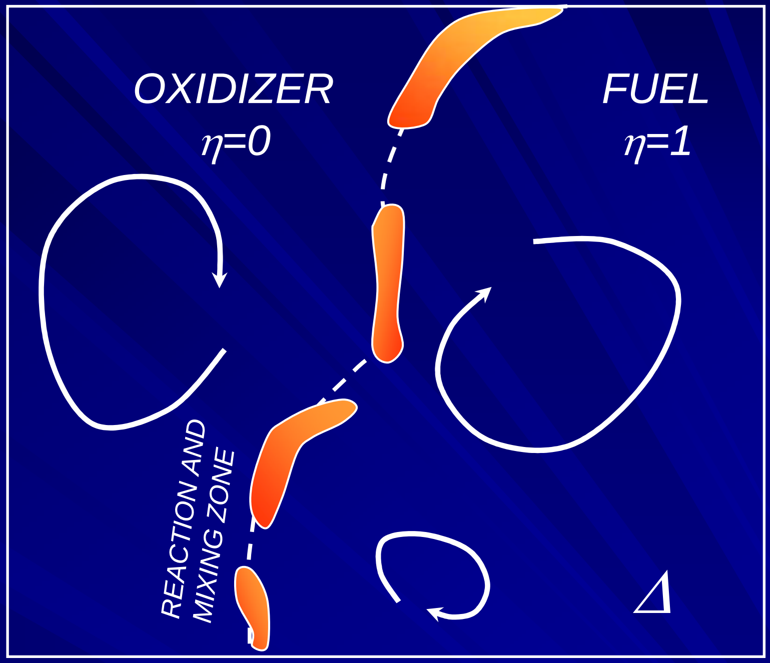
SGS Closures (Smagorinsky)

$$\tau^0_{sgs} = -2\bar{\rho}\nu_{sgs}\tilde{S}^0_{ij}$$

$$\nu_{sgs} = (C_s\Delta)^2 \left\|\tilde{S}_{ij}\right\|$$

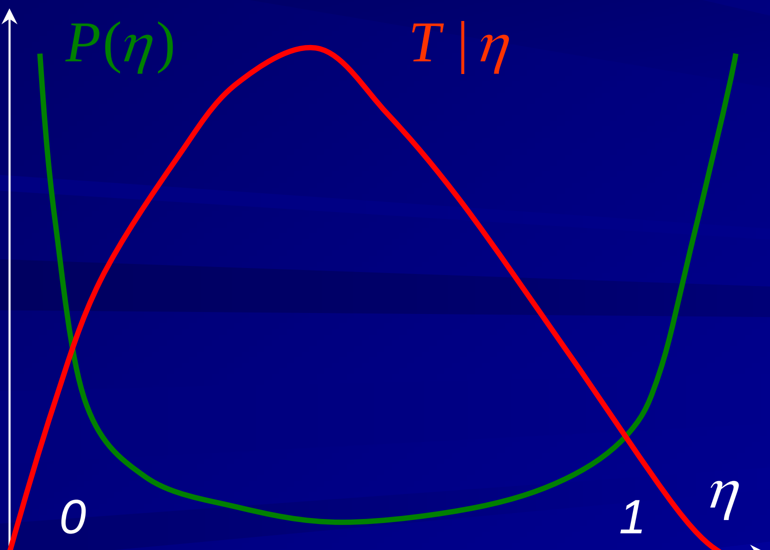
$$J^k_{sgs} = \frac{\bar{\rho}\nu_{sgs}}{Sc_t}\frac{\partial \tilde{Y}_k}{\partial x_j}$$

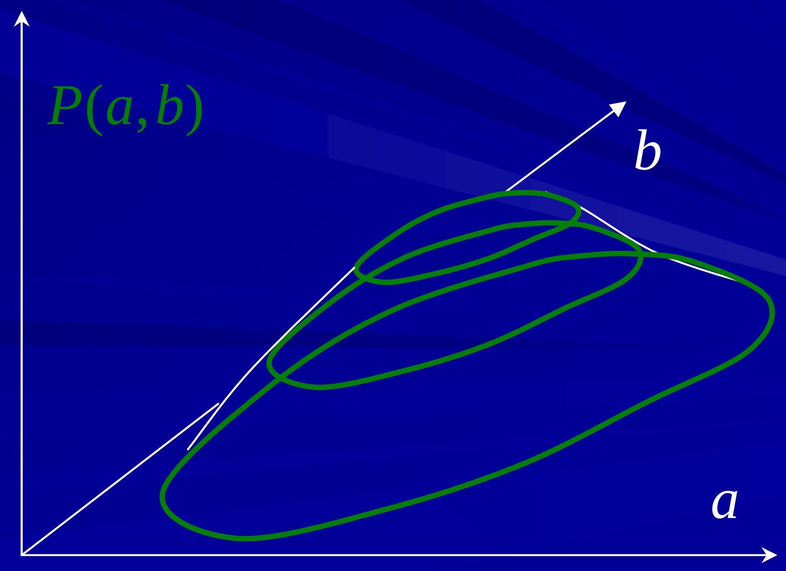




Flamelets (Peters 80's)
CMC (Klimenko, Bilger 90's)

Joint PDF (Pope 80's)





Subgrid PDF or FDF (density weighted)

Probability of observing values of the scalar in $\phi_\alpha \le Y_\alpha \le \phi_\alpha + d\phi_\alpha$

$$\overline{\rho}\, P\left(\underline{\phi}; \mathbf{x}, t\right) = \int_V \rho \prod_{k=1}^{Ns} \delta\left[\phi_k - Y_k\right] G(\mathbf{x} - \mathbf{x}'; \Delta)\, dx'$$

FDF transport equation

$$\frac{\partial \overline{\rho} P}{\partial t} + \frac{\partial \overline{\rho}\, \tilde{u}_j P}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\overline{\rho} D_{eff} \frac{\partial P}{\partial x_j}\right]$$

micromixing

$$- \frac{\partial^2}{\partial \phi_\alpha \partial \phi_\beta}\left[\overline{\rho}\left\langle D \frac{\partial Y_\alpha}{\partial x_j} \frac{\partial Y_\beta}{\partial x_j} \middle| \underline{Y} = \underline{\phi} \right\rangle P\right] - \frac{\partial}{\partial \phi_\alpha}\left[\overline{\rho}\, \omega_\alpha(\phi_\alpha)\, P\right]$$

Linear Mean Square Estimation (LMSE) or Interaction with the Mean (IEM)

$$- \frac{\partial^2}{\partial \phi_\alpha \partial \phi_\beta}\left[\overline{\rho}\left\langle D \frac{\partial Y_\alpha}{\partial x_j} \frac{\partial Y_\beta}{\partial x_j} \middle| \underline{Y} = \underline{\phi} \right\rangle P\right] = \overline{\rho} \beta \frac{\partial}{\partial \phi_\alpha}\left[\left(\phi_\alpha - \tilde{Y}_\alpha\right) P\right]$$

SGS frequency

$$\beta \approx C_D \frac{\nu + \nu_{sgs}}{\Delta^2}$$

Eulerian Monte Carlo Field (Valiño 1998)

*PDF represented as ensemble of **Stochastic Fields (SF)***

$$P(\underline{\phi};\mathbf{x},t)=\frac{1}{N_f}\sum_{n=1}^{N_f}\prod_{k=1}^{N_s}\delta\left[\phi_k-\zeta_k^n(\mathbf{x},t)\right] \qquad \tilde{Y}_k=\frac{1}{N_f}\sum_{n=1}^{N_f}\zeta_k^n$$

Transport equation of stochastic fields (SPDE)

$$\underbrace{\frac{\partial\bar{\rho}\zeta_k^n}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j\zeta_k^n}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}D_{eff}\frac{\partial\zeta_k^n}{\partial x_j}\right)}+\omega_k\left(\zeta_k^n\right)+\underbrace{\left(\frac{2D_{eff}}{\Delta t^2}\right)^{1/2}\frac{\partial\zeta_k^n}{\partial x_j}dW_j^n}\underbrace{-\frac{\bar{\rho}\beta}{2}\left(\zeta_k^n-\tilde{Y}_k\right)}$$

Convection-Diffusion | Source term | Stochastic | IEM

Summary SF model

Pros

(vs. Lagrangian PDF)

Easy to implement
Statistics easy to obtain
No interpolation error

(vs. assumed PDF models)

More physics
No assumptions chem-turbulence

Cons

(vs. Lagrangian PDF)

Spatial discretization error

(vs. assumed PDF models)

Cost
Statistical error , N_f low

Mueller-H_2 Mechanism

9 species
19 reactions

Reaction Number		*A* *mol cm s K*	*b*	*E* *cal mol^{-1}*
H_2/O_2 Chain Reactions				
1	$H + O_2 \leftrightarrow O + OH$	1.9E+14	0.	16439
2	$O + H_2 \leftrightarrow H + OH$	0.508E+05	2.67	6290
3	$H_2 + OH \leftrightarrow H_2O + H$	0.216E+09	1.51	3430
4	$O + H_2O \leftrightarrow OH + OH$	2.97E+06	2.02	13400
Dissociation/Recombination H_2/O_2				
5	$H_2 + M \leftrightarrow H + H + M$	4.577E+19	-1.4	104380
6	$O + O + M \leftrightarrow O_2 + M$	6.165E+15	-0.5	0
7	$O + H + M \leftrightarrow OH + M$	4.714E+18	-1	0
8	$H + OH + M \leftrightarrow H_2O + M$	2.21E+22	-2	0
Formation and consumption HO_2/H_2O_2				
9	$H + O_2 + M \leftrightarrow HO_2 + M$	1.475E+12	0.	823
10	$HO_2 + H \leftrightarrow H_2 + O_2$	1.66E+13	0.	295
11	$HO_2 + H \leftrightarrow OH + OH$	7.079E+13	0.	0
12	$HO_2 + O \leftrightarrow O_2 + OH$	0.325E+14	0.	-497
13	$HO_2 + OH \leftrightarrow H_2O + O_2$	2.89E+13	0.	11982
14	$HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2$	4.2E+14	0.	-1629
15	$H_2O_2 + M \leftrightarrow OH + OH + M$	2.951E+14	0.	48430
16	$H_2O_2 + H \leftrightarrow H_2O + OH$	0.241E+14	0.	3970
17	$H_2O_2 + H \leftrightarrow HO_2 + H_2$	0.482E+14	2.	7950
18	$H_2O_2 + O \leftrightarrow OH + HO_2$	9.55E+06	0.	3970
19	$H_2O_2 + OH \leftrightarrow HO_2 + H_2O$	5.8E+14	0.	0

Test Case I (Markides)

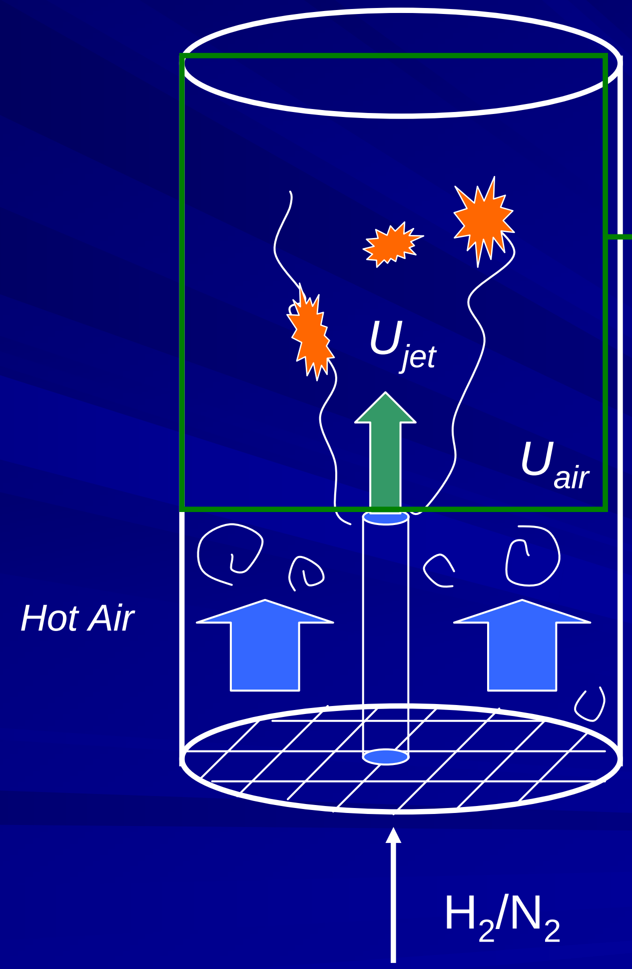
T_{air} = 960-1000 K
T_{jet} = 750 K

U_{jet} = 26-120 m/s
U_{air} = 26 m/s

d_{jet} = 2.25 mm
l_{grid} = 3 mm

Re_t = 90-160

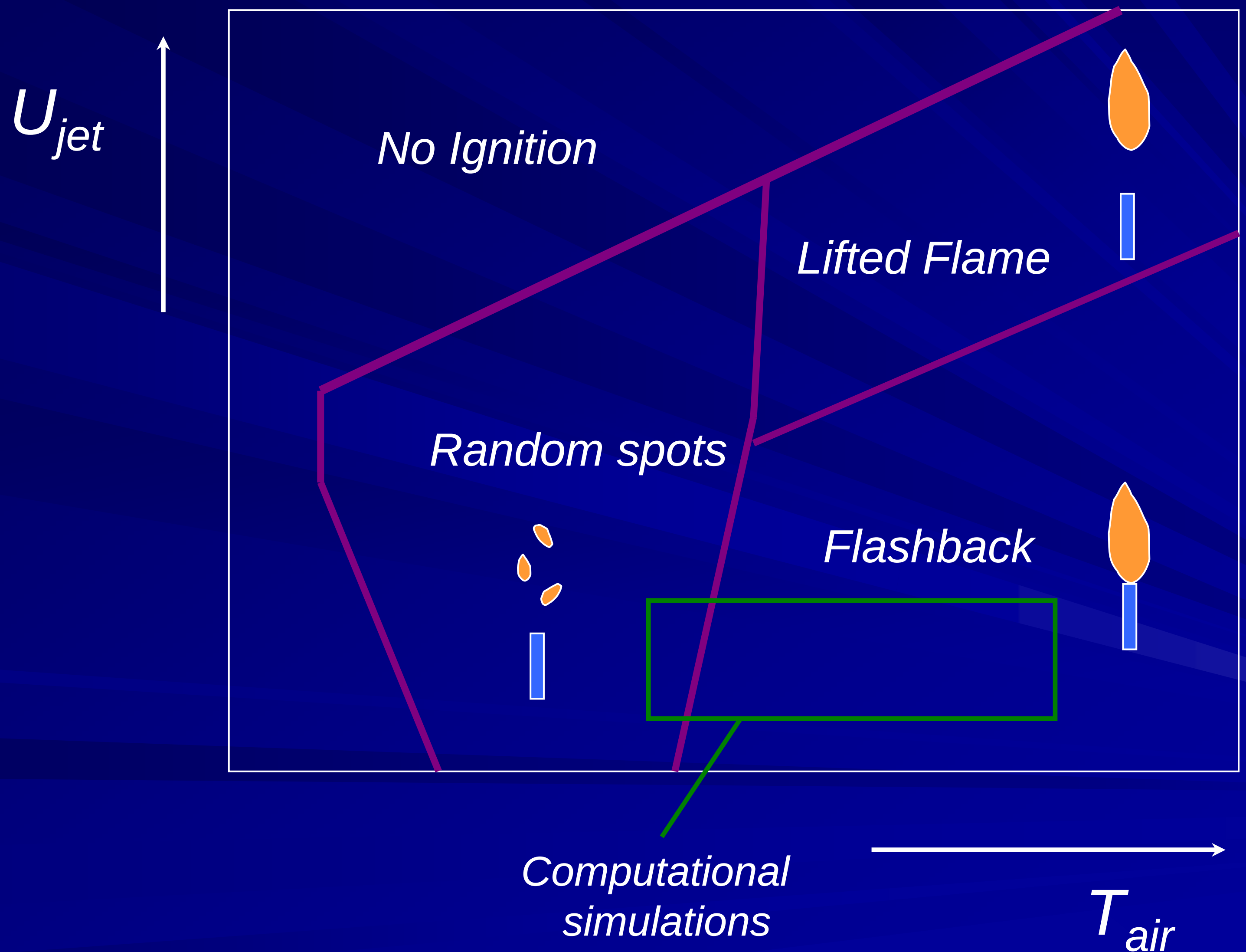
<u>Jet</u>
$Y(N_2)=0.87$
$Y(H_2)=0.13$



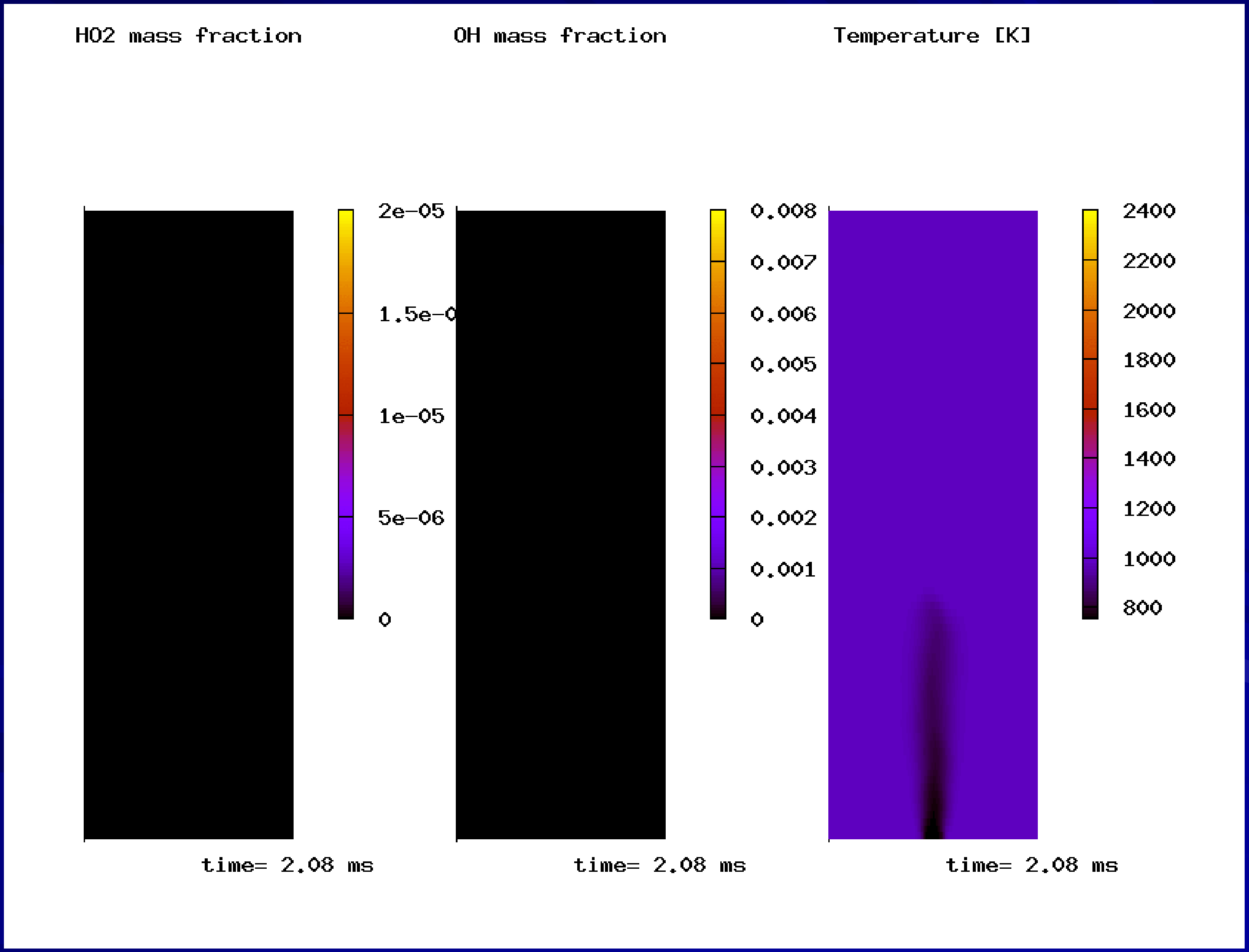
160 x 70 x 48 (Cylindrical)
Nfields=8

<u>Inflow BC</u>
Synthetic turbulence
Klein *et al.* (1998)

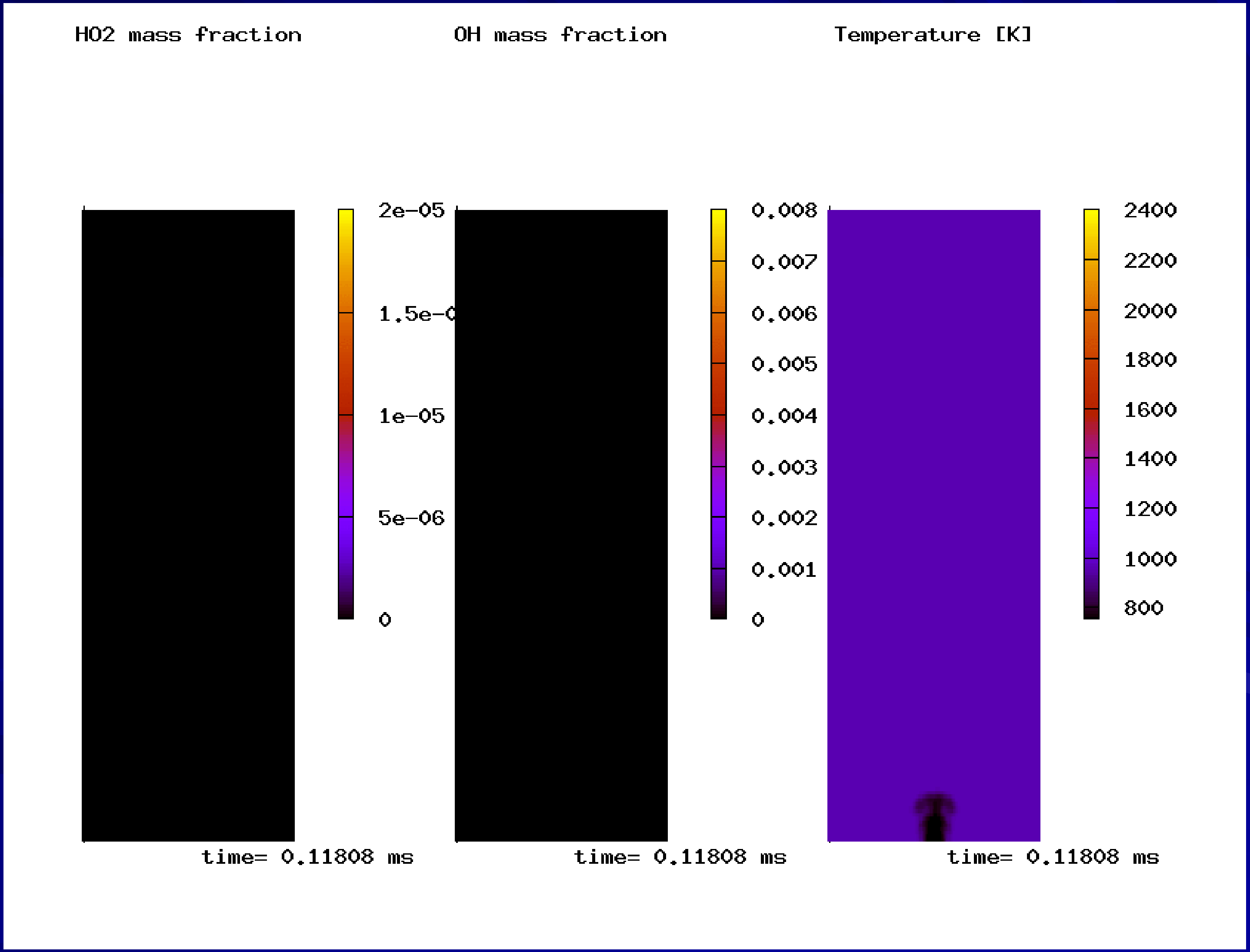
Bulk behaviour

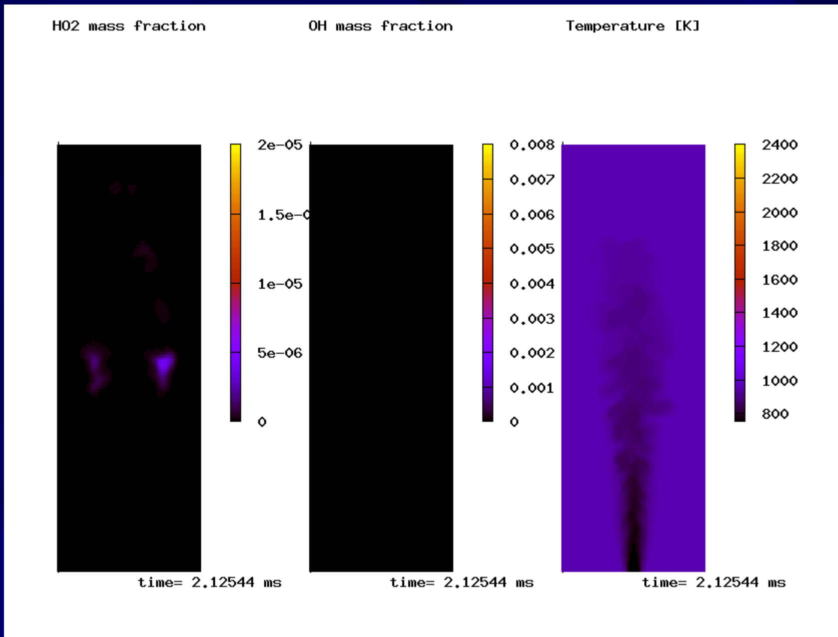


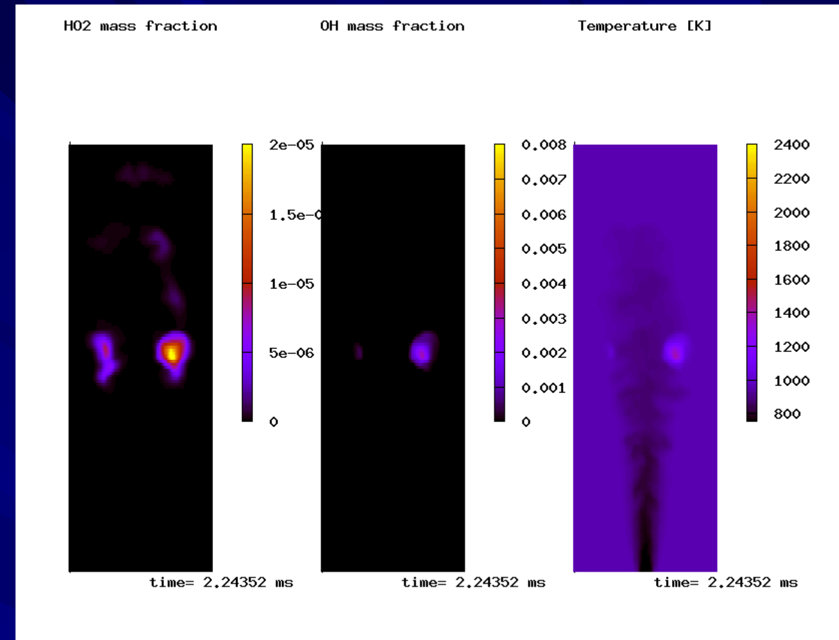
Animation (U=26 m/s T=960 K)

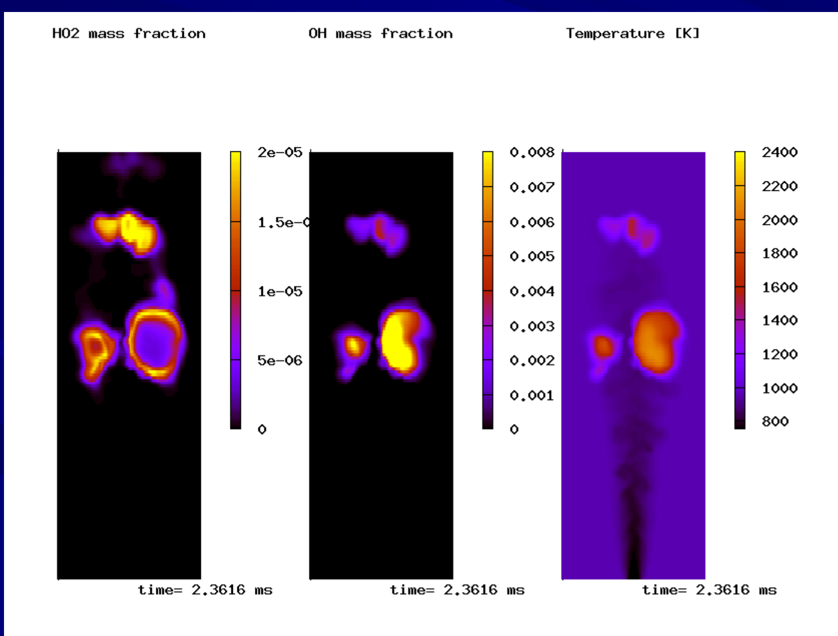


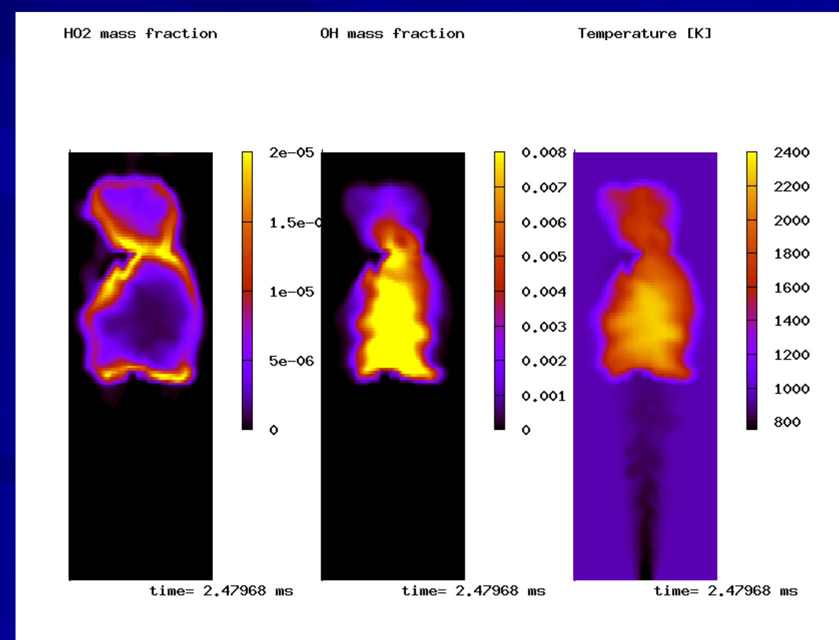
Animation (U=70 m/s T=960 K)




HO2 mass fraction
OH mass fraction
Temperature [K]
2e-05
1.5e-0
1e-05
5e-06
0
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
2400
2200
2000
1800
1600
1400
1200
1000
800
time= 2.12544 ms
time= 2.12544 ms
time= 2.12544 ms

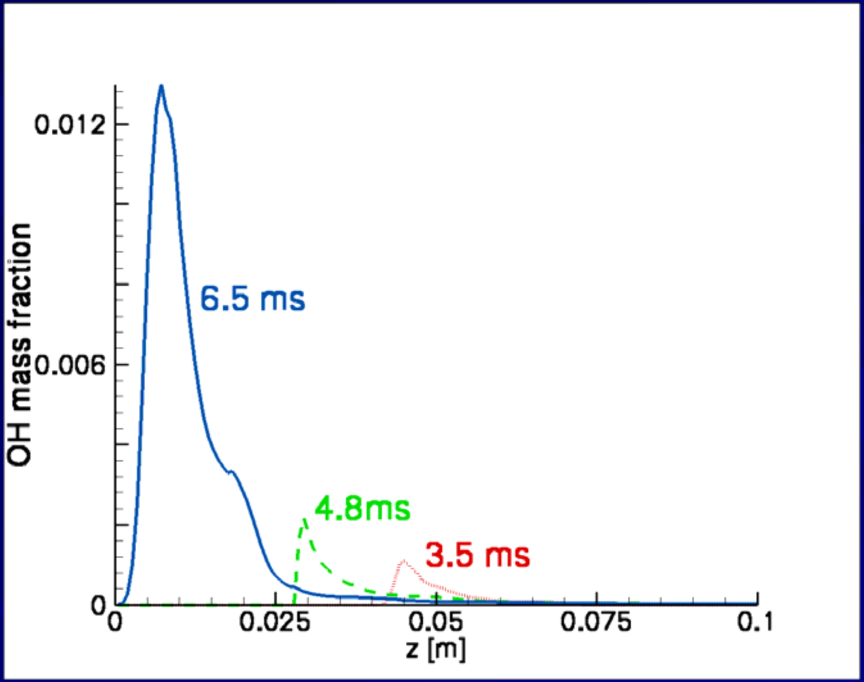

HO2 mass fraction
OH mass fraction
Temperature [K]
2e-05
1.5e-0
1e-05
5e-06
0
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
2400
2200
2000
1800
1600
1400
1200
1000
800
time= 2.24352 ms
time= 2.24352 ms
time= 2.24352 ms

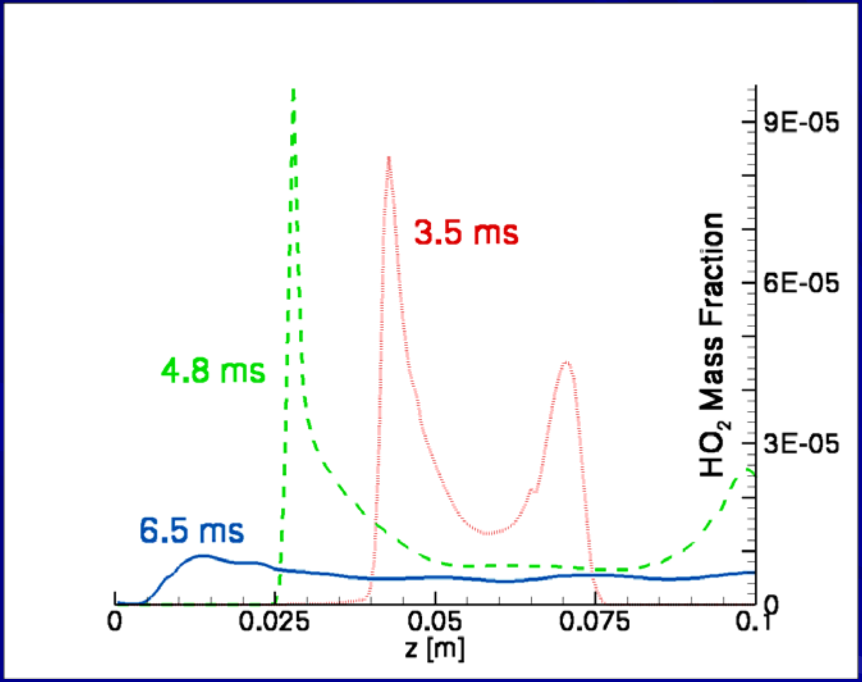

HO2 mass fraction
OH mass fraction
Temperature [K]
2e-05
1.5e-0
1e-05
5e-06
0
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
2400
2200
2000
1800
1600
1400
1200
1000
800
time= 2.3616 ms
time= 2.3616 ms
time= 2.3616 ms


HO2 mass fraction
OH mass fraction
Temperature [K]
2e-05
1.5e-0
1e-05
5e-06
0
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
2400
2200
2000
1800
1600
1400
1200
1000
800
time= 2.47968 ms
time= 2.47968 ms
time= 2.47968 ms

Results I

U_{jet}=26 m/s T=960 K

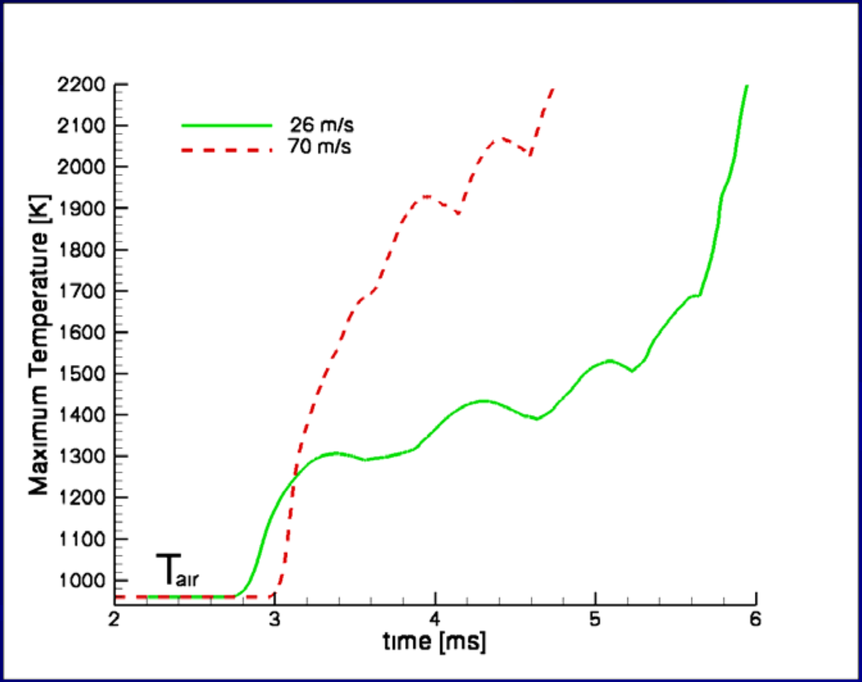


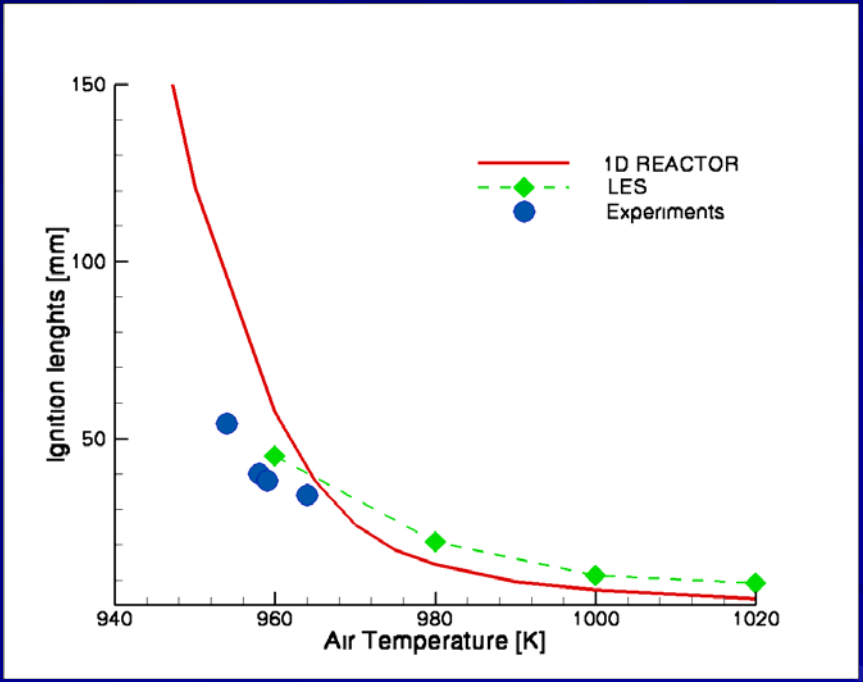


OH

HO_2

Results II



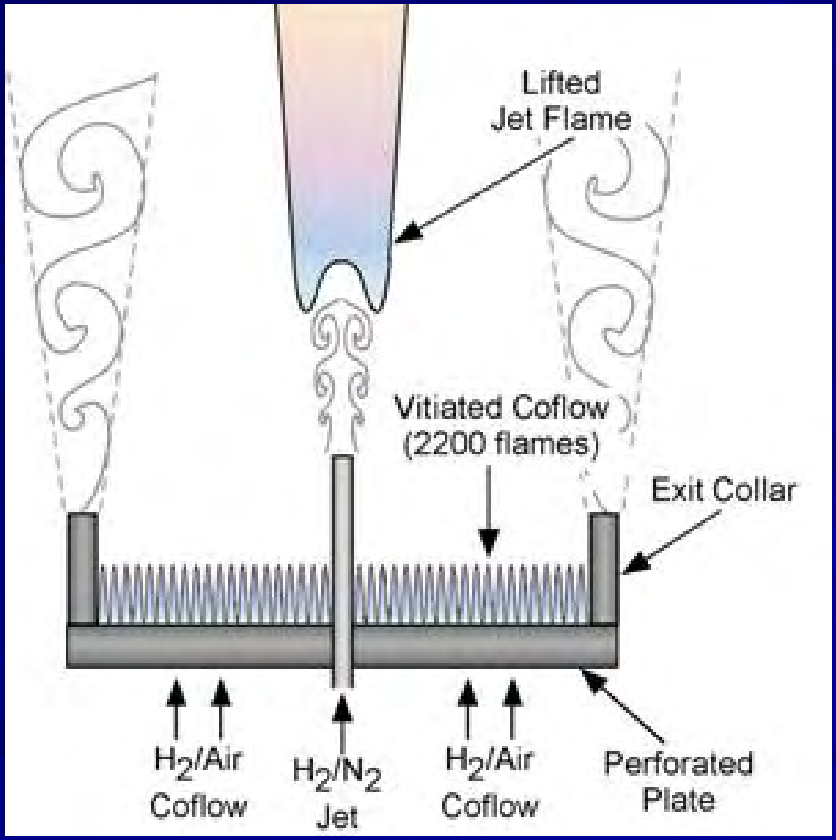


Maximum T

Ignition Length

Test-Case II (Cabra flame)

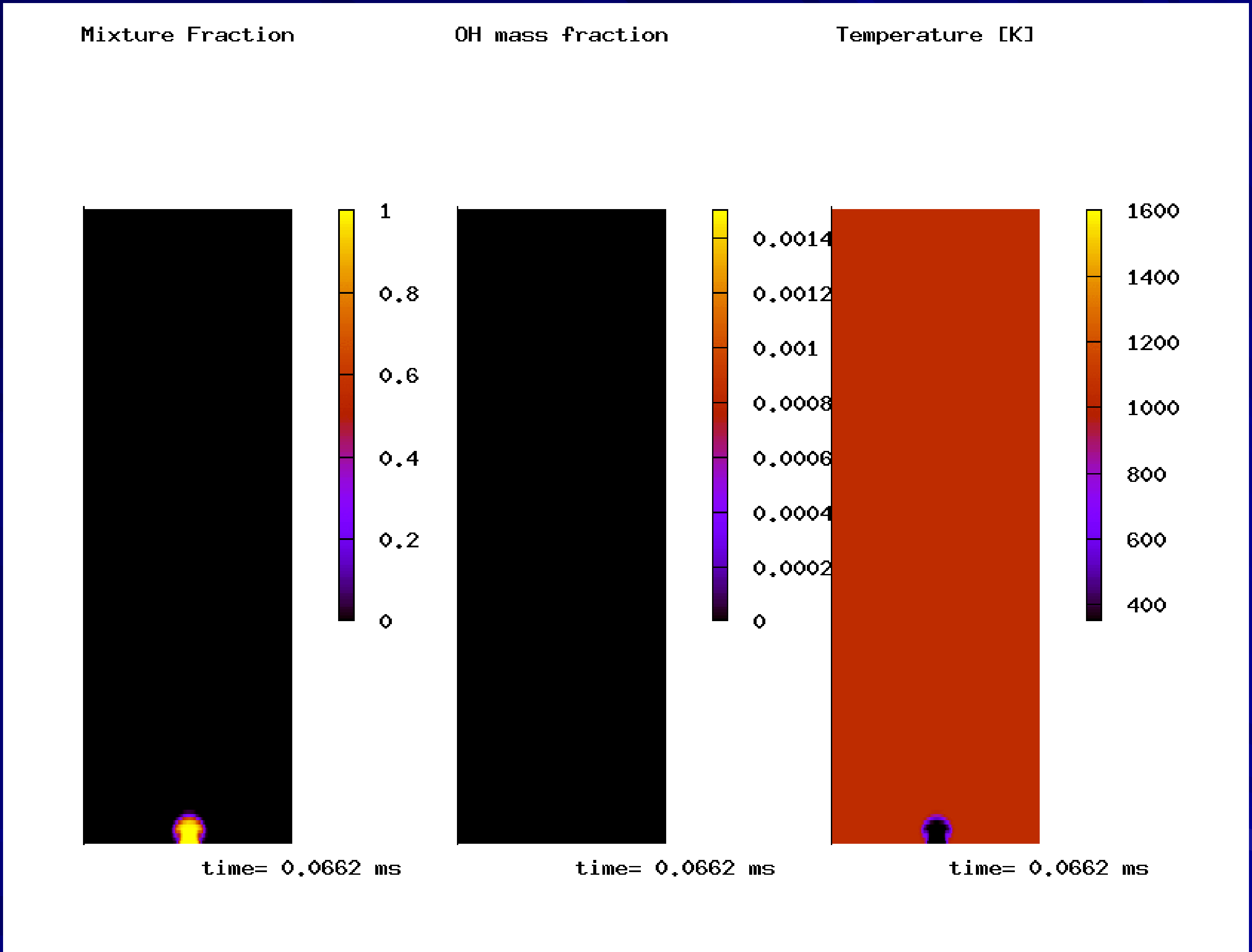
V_{jet} = 107 m/s
V_{air} = 3.5 m/s
T_{jet} = 305 K
T_{air} = 1045 K
Re = 23650
D= 4.57 mm
Air
$X(O_2)$=0.147
$X(N_2)$=0.7532
$X(H_2O)$=0.0989
Jet
$X(N_2)$=0.75
$X(H_2)$=0.25



Grid (cylindrical)
coarse
160 × 80 × 48

PDF
8-16 fields

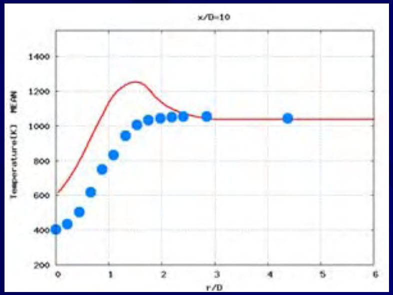
CPU Cost
(coarse 8 fields)
PDF 960 CPUh

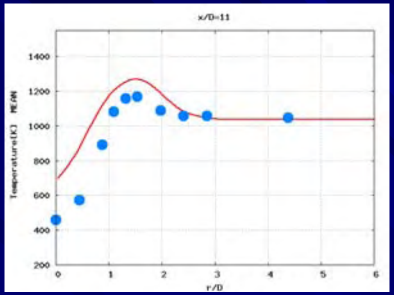

Mixture Fraction
OH mass fraction
Temperature [K]
1
0.8
0.6
0.4
0.2
0
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
1600
1400
1200
1000
800
600
400
time= 0.0662 ms
time= 0.0662 ms
time= 0.0662 ms

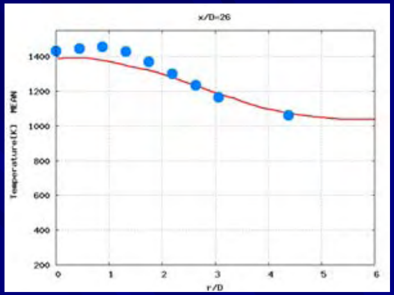
LES-PDF

T [K]

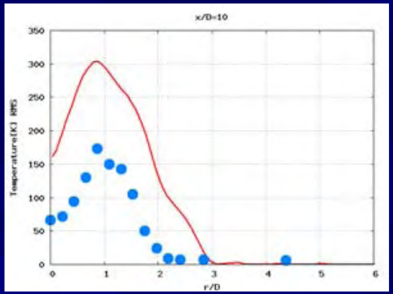
MEAN

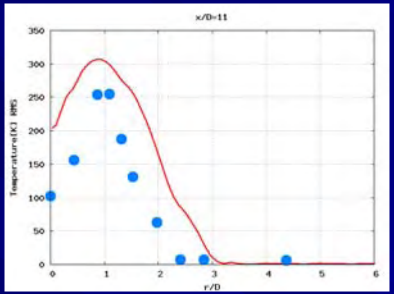


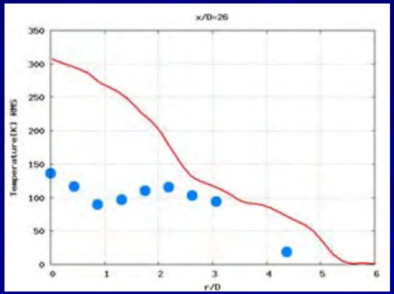




RMS

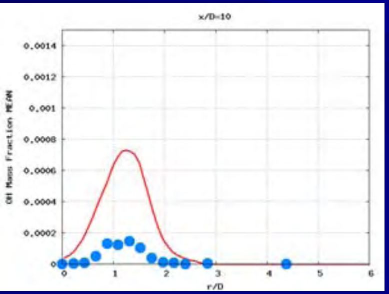


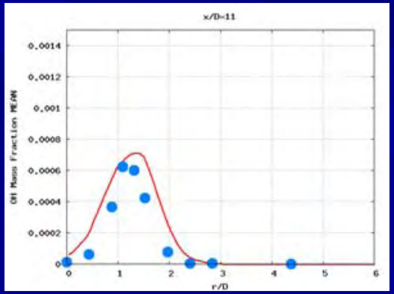


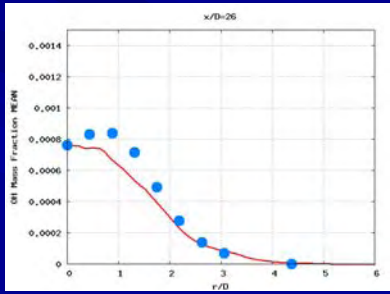


OH

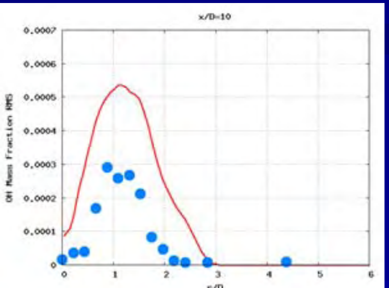
MEAN

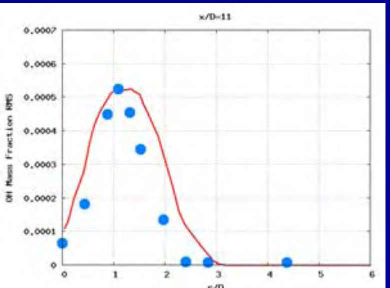


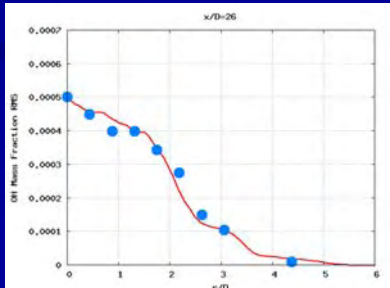




RMS







Conclusions

- Model capable, “acceptable” results
- Random spot regime elusive

  Increase Number of fields
- *Very sensitive to air Temperature errors.*

  Few experimental data