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# Large-Eddy Simulation of Pulverised Coal Combustion

# Background: PsiPhi

Inhouse Code, Kempf Group

- ✦ We develop C-LES since 1999
- ✦ PsiPhi since 2007
- ✦ Optimised for LES and DNS
- ✦ Massively parallel ( $2^{15}$  cores)
- ✦ Gas, spray, coal flames
- ✦ Nano particle synthesis
- ✦ Engine simulations



Pseudo X-Ray



Section



Pseudo X-Ray



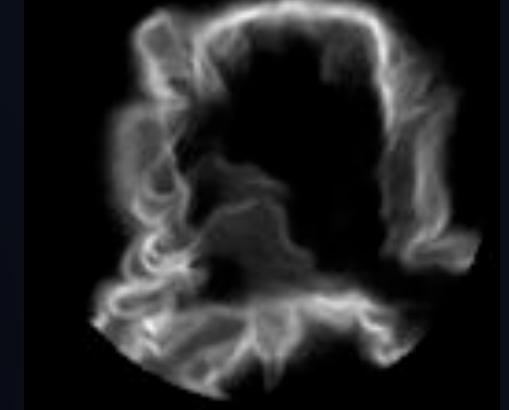
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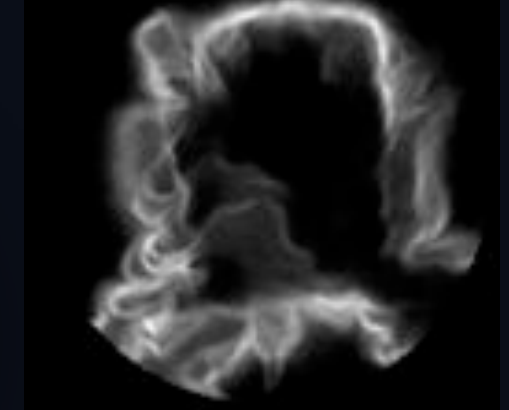
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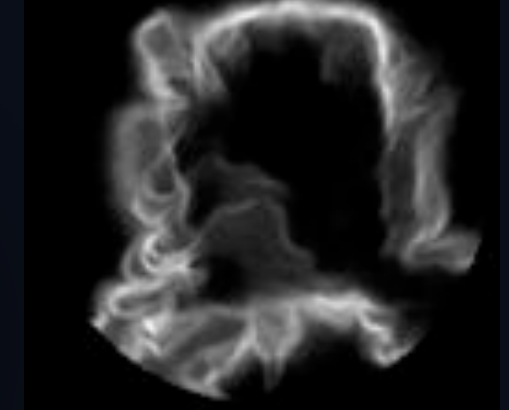
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# Background: LES

Large-Eddy Simulation vs. RANS (classical CFD)

## ✦ RANS

- ✦ Time-averaged, steady
- ✦ „*Photo, long exposure*“ ➡
- ✦ All turbulent fluctuations must be modelled.
- ✦ Correlations of fluctuations must also be modelled! ➡
- ✦ Closure models matter!
- ✦ Numerics matter little.

## ✦ LES

- ✦ Locally filtered, unsteady
- ✦ „*Movie, slightly blurred*“
- ✦ Strong fluctuations are calculated.
- ✦ Correlations of strong fluctuations just calculated.
- ✦ Closure models matter little.
- ✦ Accurate numerics needed!

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Large-Eddy Simulation



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RANS (steady)



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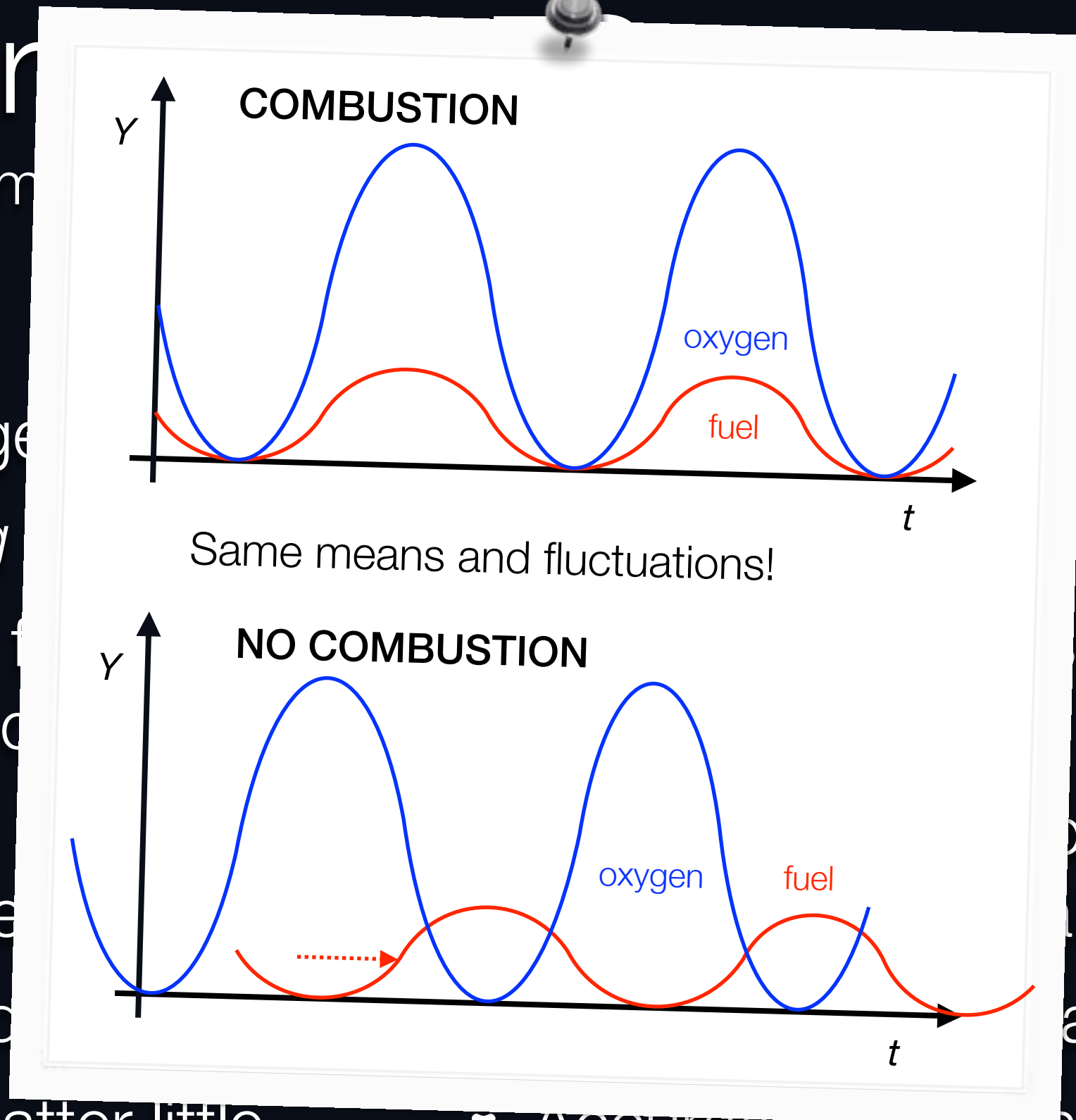


# Background

Large-Eddy Simulation

## ❖ RANS

- ❖ Time-averaged
- ❖ „Photo, long exposure“
- ❖ All turbulent fluctuations are averaged out
- ❖ All turbulent fluctuations must be modeled
- ❖ Correlations must also be modeled
- ❖ Closure models
- ❖ Numerics matter little.
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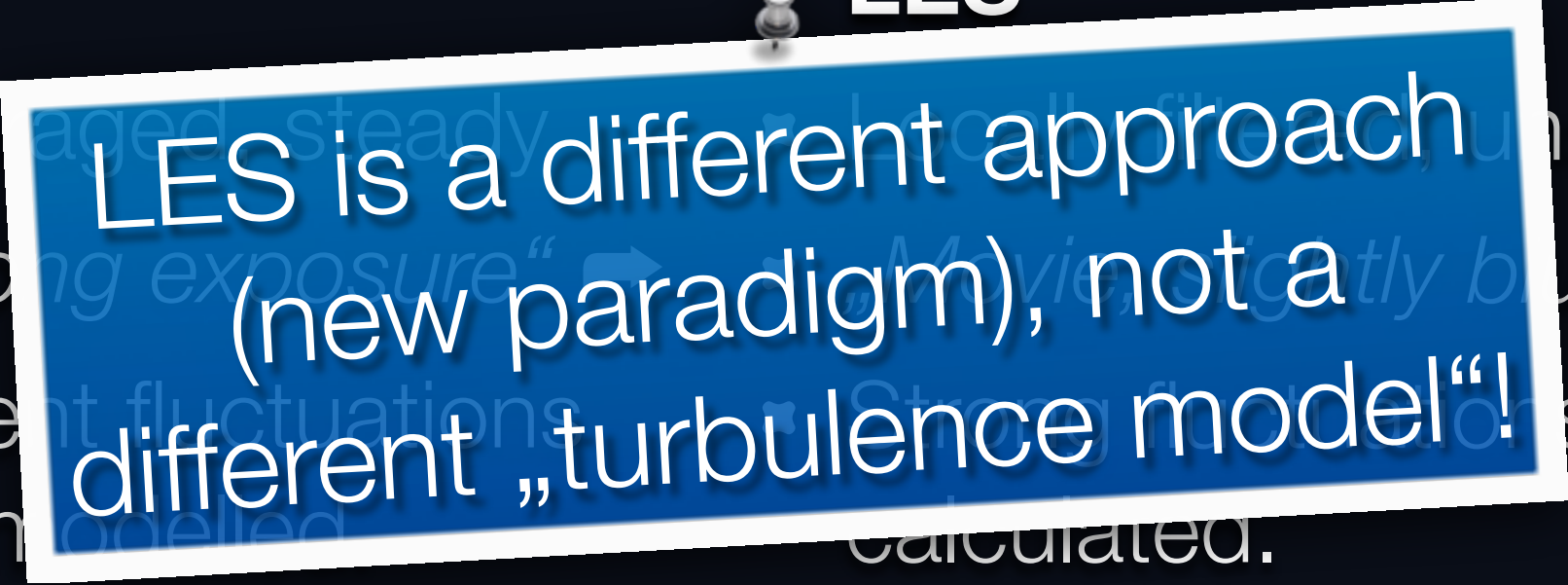
# Background: LES

Large-Eddy Simulation vs. RANS (classical CFD)

## ✦ RANS

- ✦ Time-averaged, steady
- ✦ „Photo, long exposure“
- ✦ All turbulent fluctuations must be modelled

## ✦ LES

- 
- ✦ LES is a different approach (new paradigm), not a different „turbulence model“!
  - ✦ Correlations of strong fluctuations just calculated.
  - ✦ Closure models matter little.
  - ✦ Accurate numerics needed!

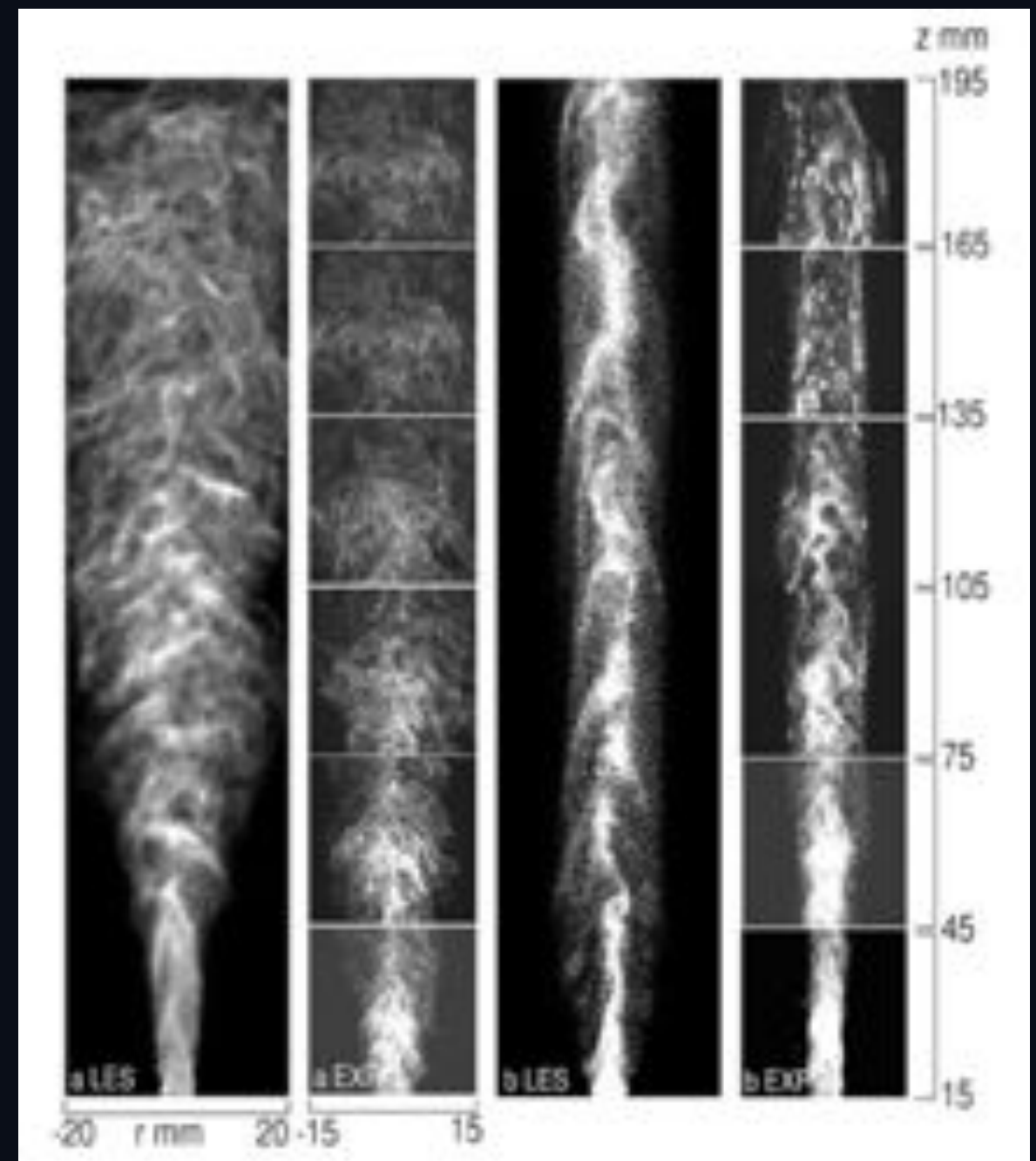
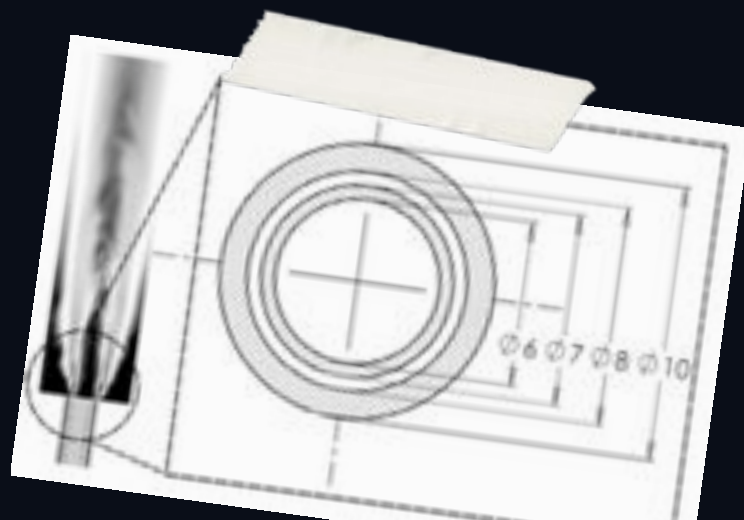
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# CRIEPI Burner

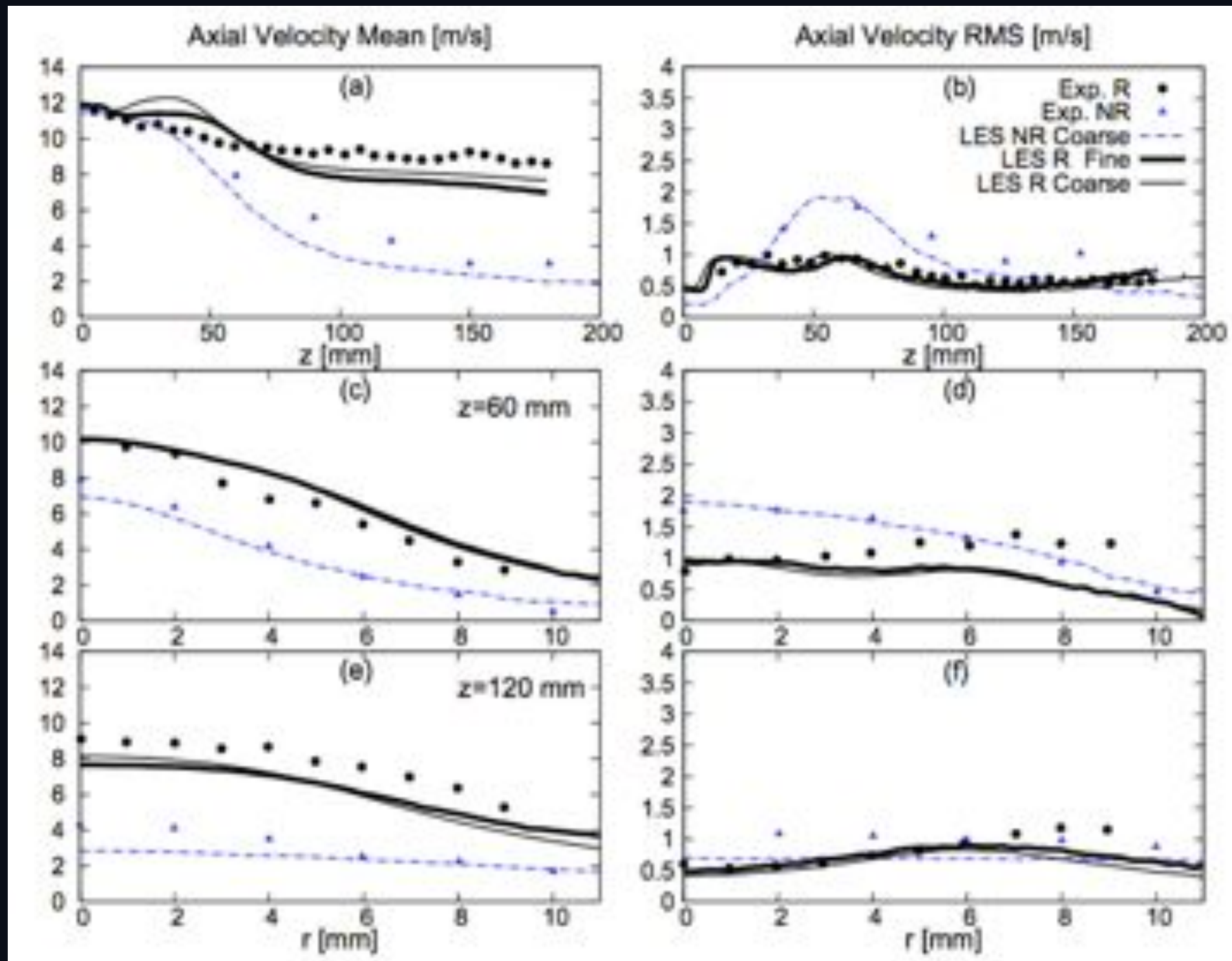
Franchetti, B.M., Cavallo Marincola, F., Navarro-Martinez, S, Kempf, A.M, Large Eddy Simulation of a Pulverised Coal Jet Flame, Proc. Combust. Inst. 34 (2013) 2419-2426.

- ✦ Small scale jet burner
- ✦ Coal: 0.149 g/s
- ✦ Methane pilot, 23 cm<sup>3</sup>/s
- ✦  $Re \approx 2300$
- ✦  $10^7$  computational cells
- ✦ Euler-Lagrange LES

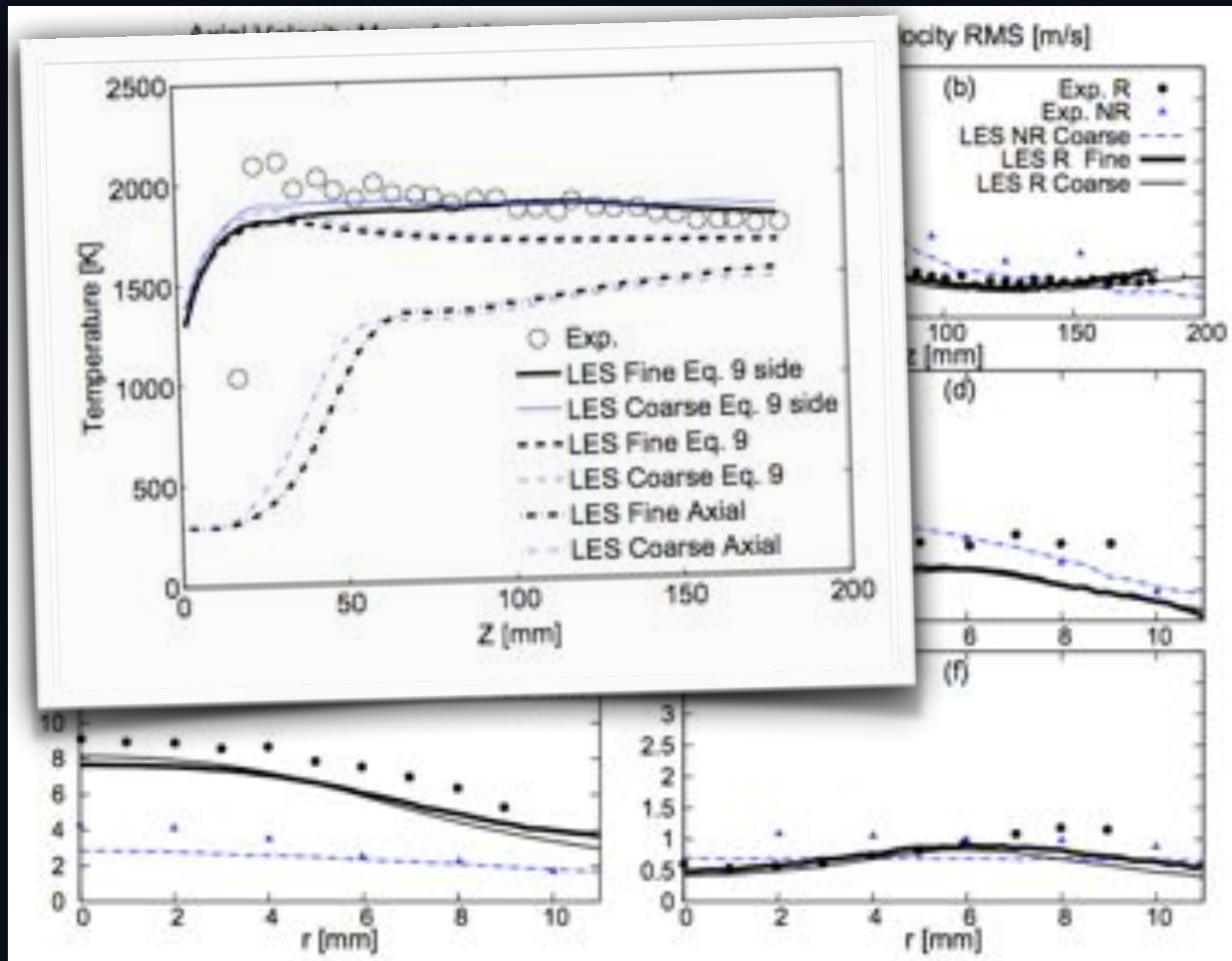




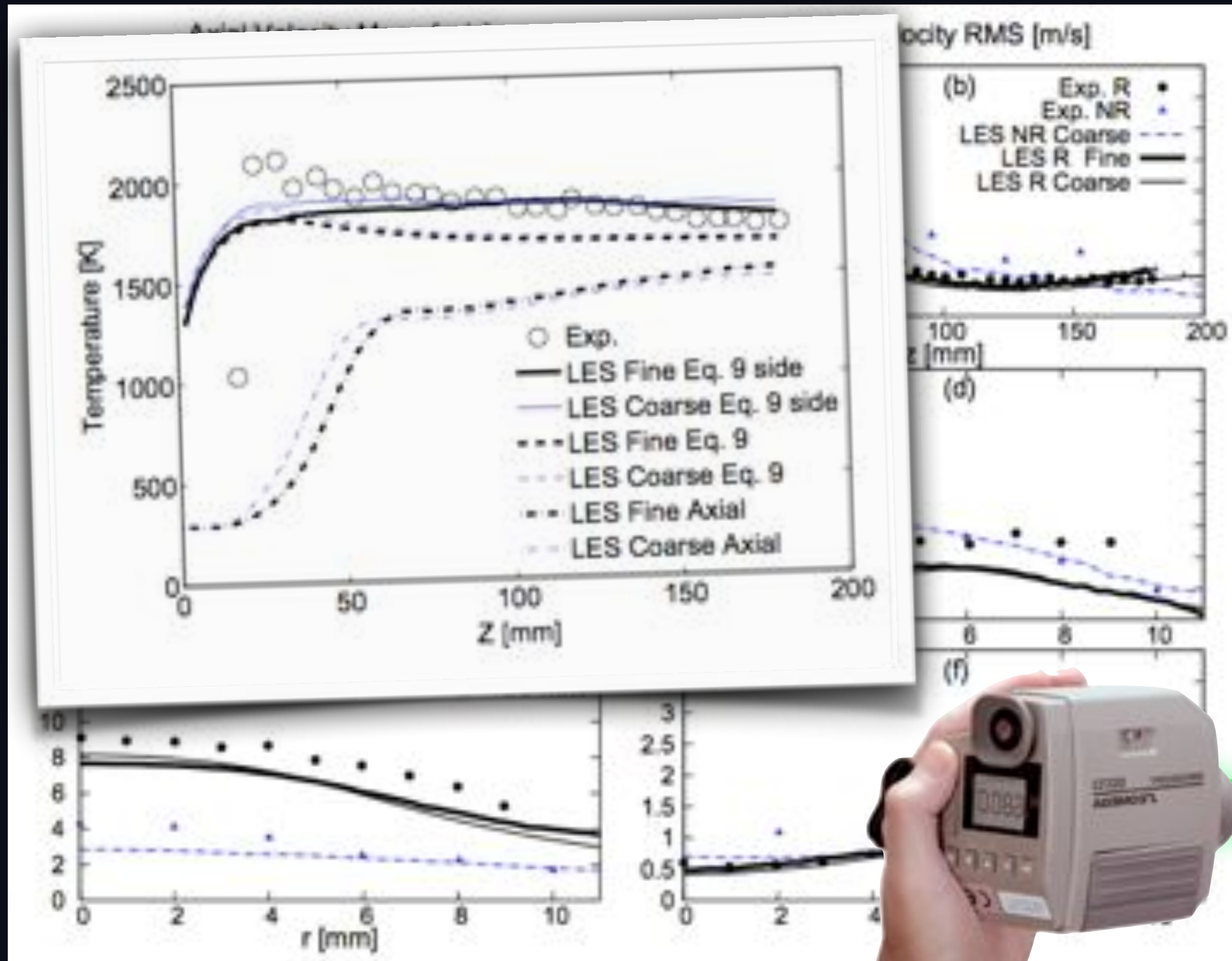
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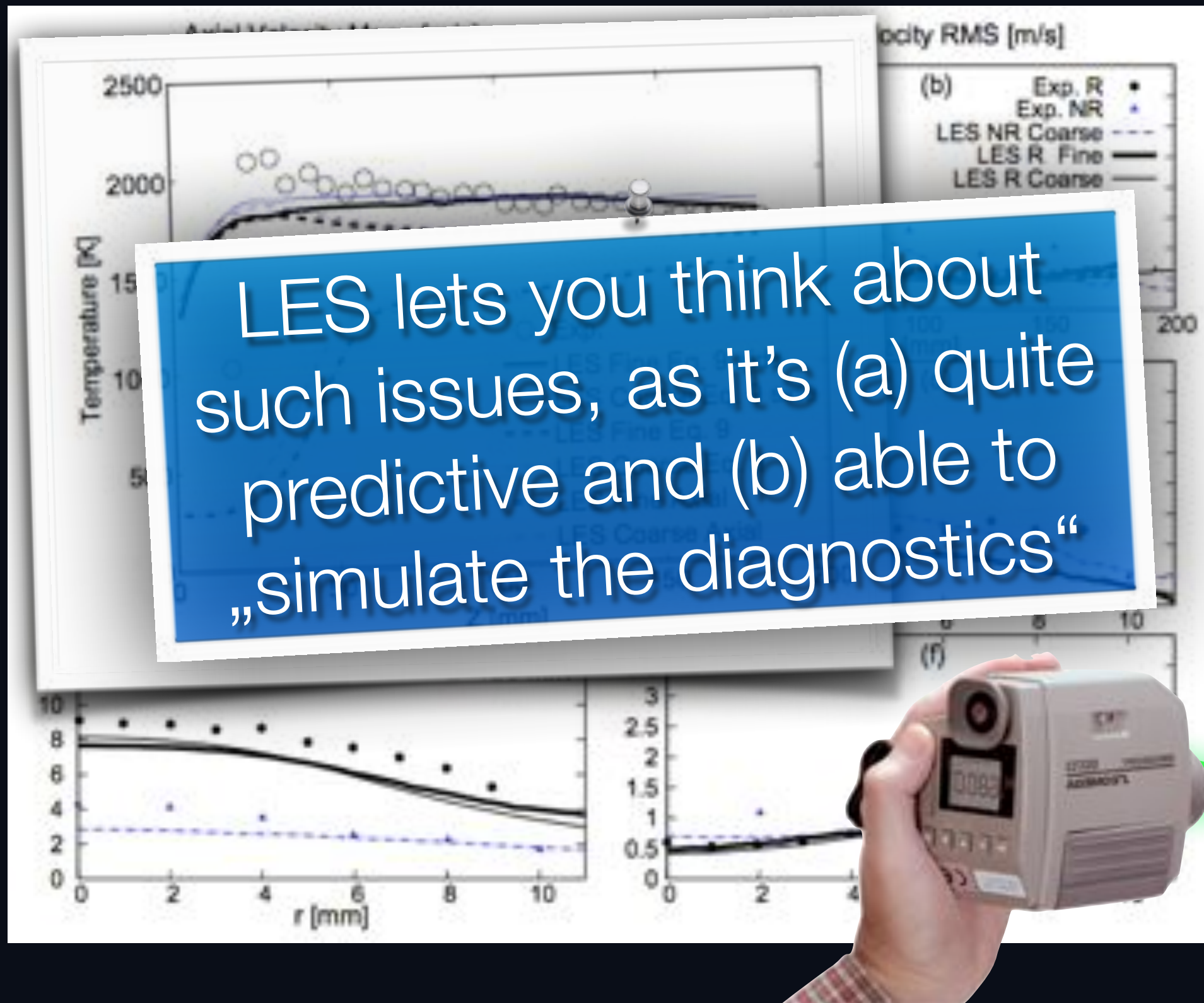


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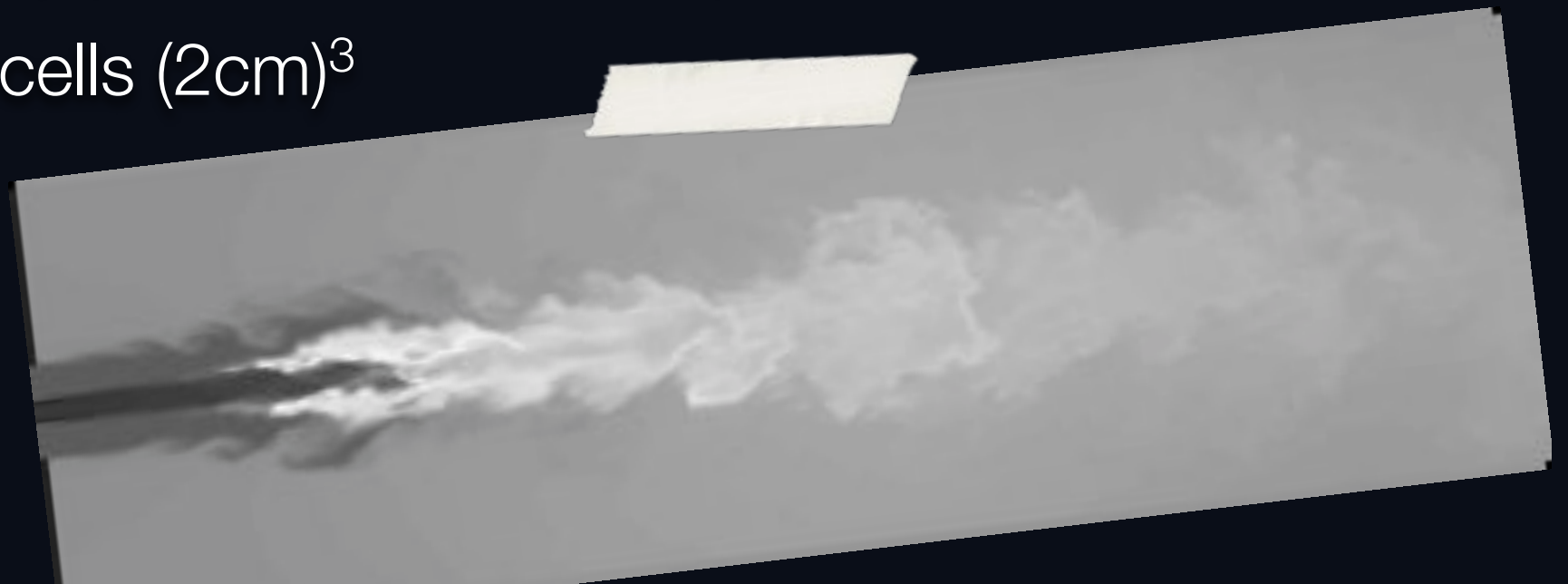


# IFRF Flame B1

- ✦ Primary:  $d=0.07\text{m}$ ,  $40.7\text{m/s}$ ,  $212\text{kg/h}$ ,  $463\text{K}$
- ✦ Secondary:  $d=0.2\text{m}$ ,  $9.6\text{m/s}$ ,  $773\text{K}$
- ✦ Turbulence: Smagorinsky
- ✦ Postulate substance
- ✦ Devolatilisation: First order single rate (Badzioch, Hawksley)
- ✦ Char combustion: Intrinsic reaction rate model (Smith)
- ✦ Radiation: DOM, (grey products, volatiles), particles scatter
- ✦ Mesh:  $2.8\text{M} / 6.7\text{M}$  cells  $(2\text{cm})^3$

Proximate Analysis		[% wt.]
Fixed Carbon		59.5
Volatiles		31
Ash		7.5
Moisture		2
Ultimate Analysis		[% wt.]
C		74.65
H		4.7
O		11.08
N		1.12
S		0.85

J.B. Michel, R. Payne. Detailed measurements of long pulverized coal flames for the characterisation of pollutant formation. Tech. Report, IFRF, 1980.

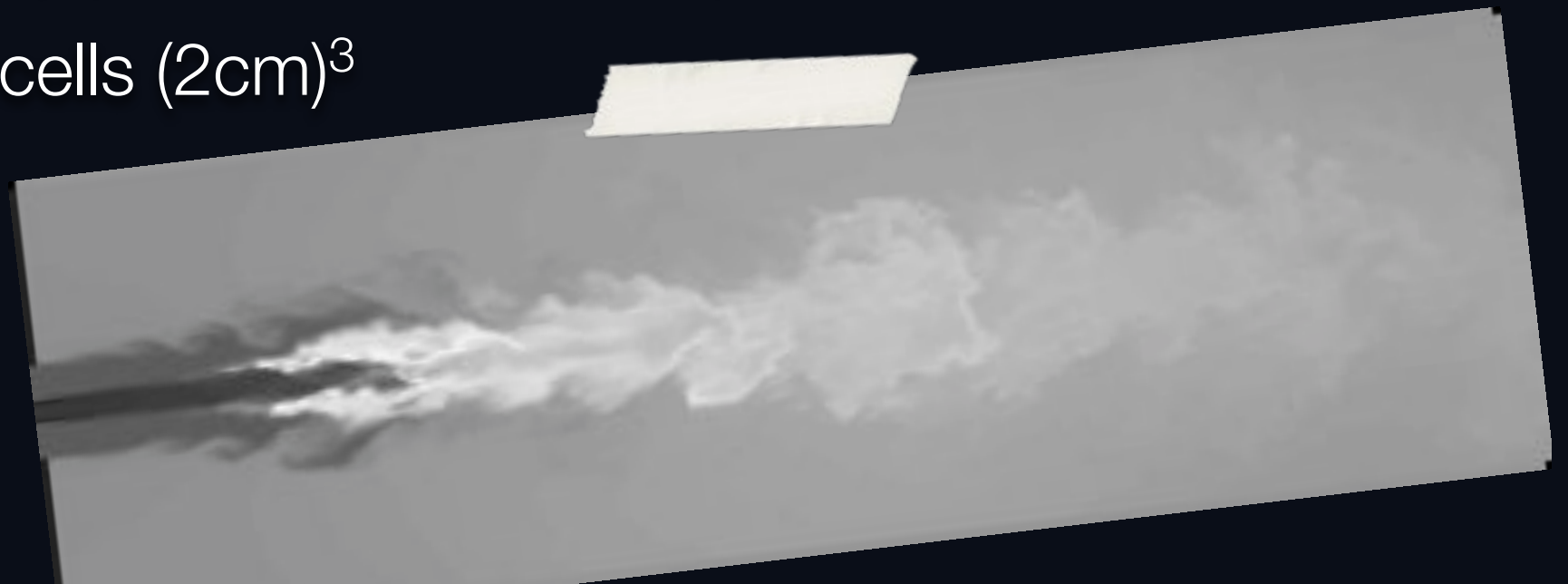


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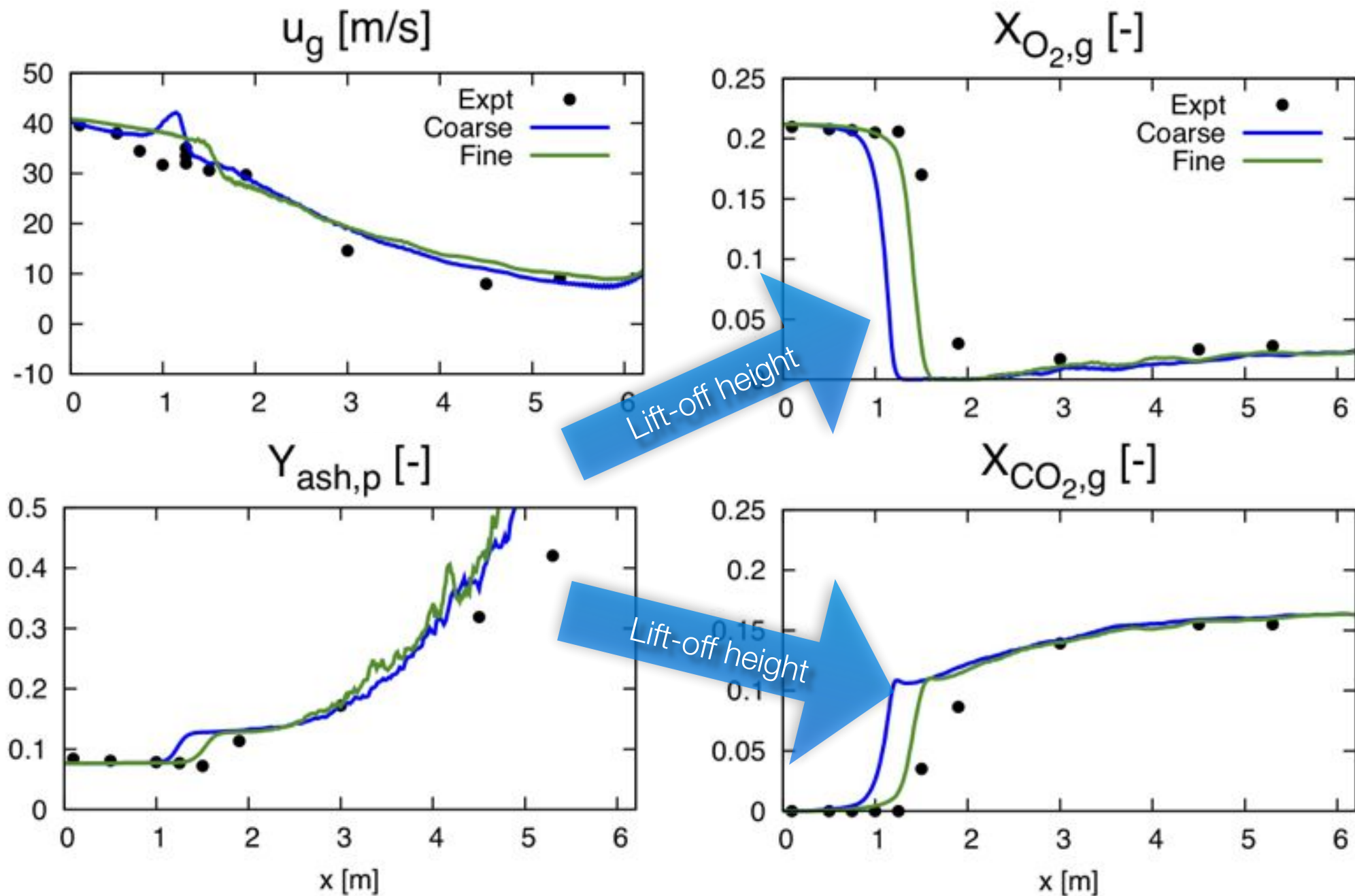
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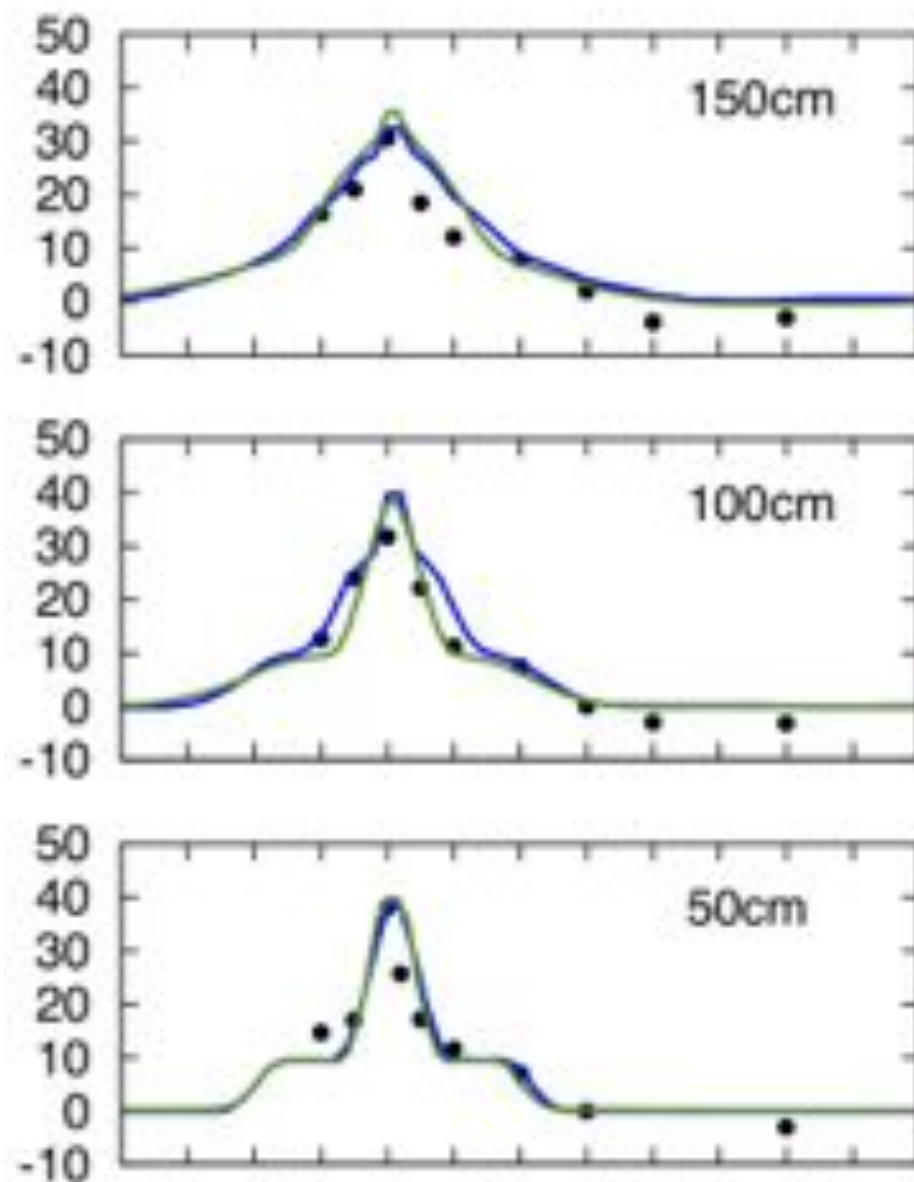
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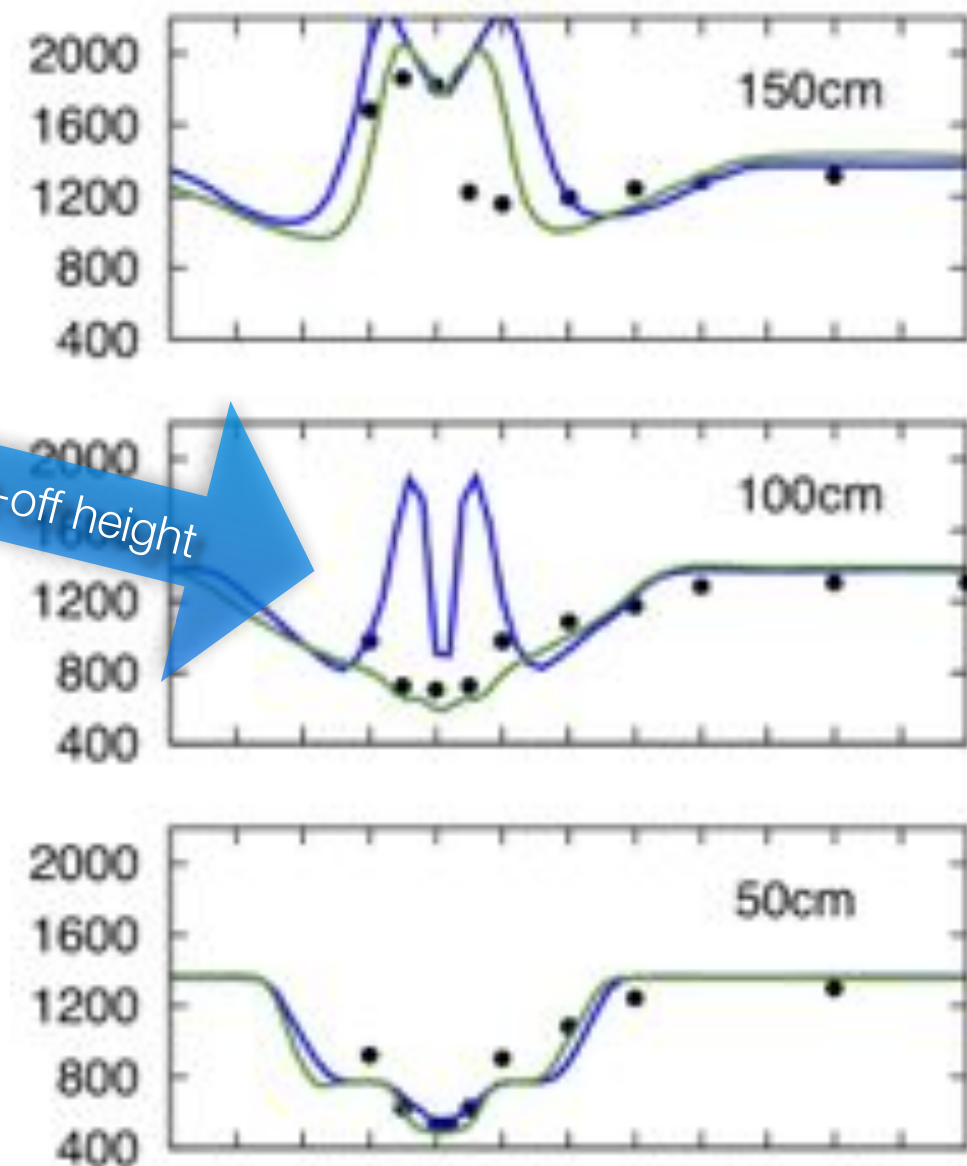


# IFRF Flame B1

Mean axial velocity



Temperature

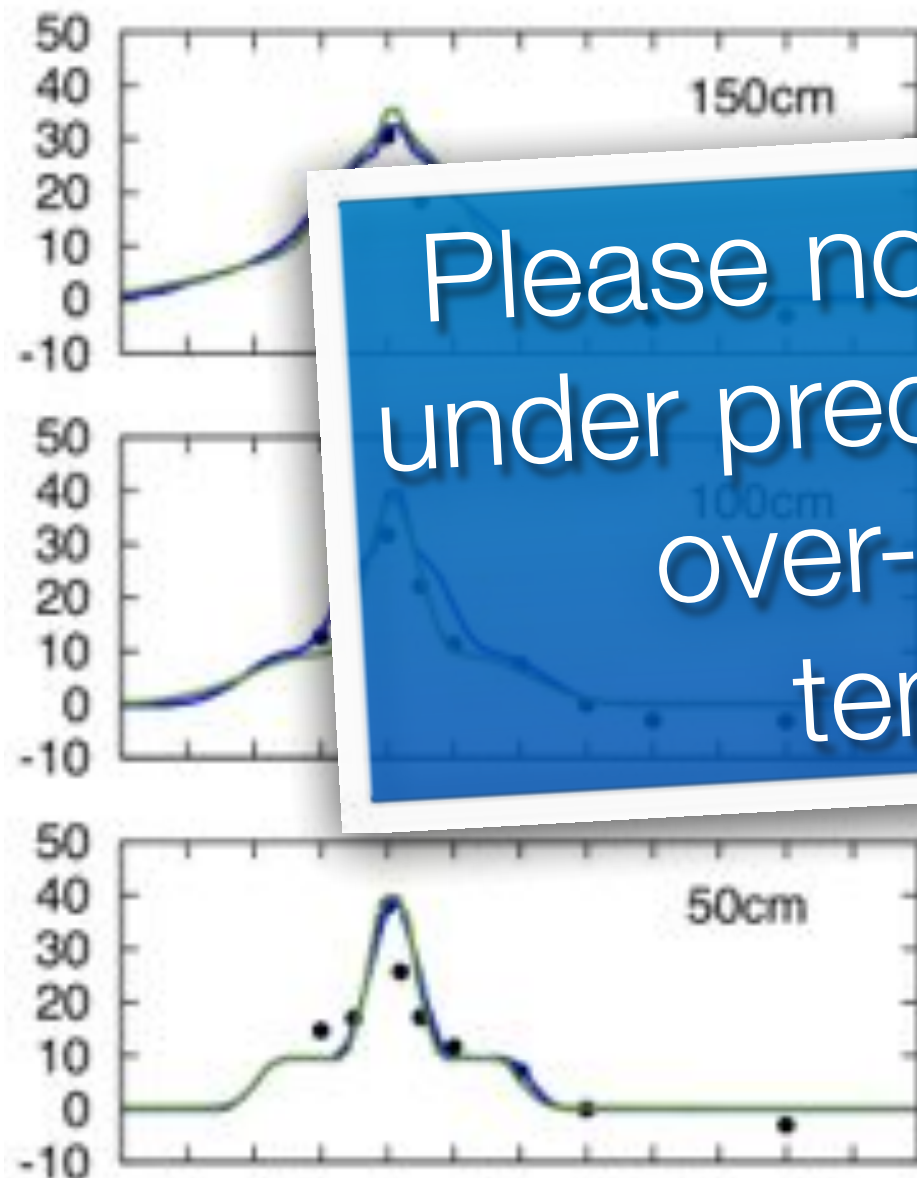


Lift-off height

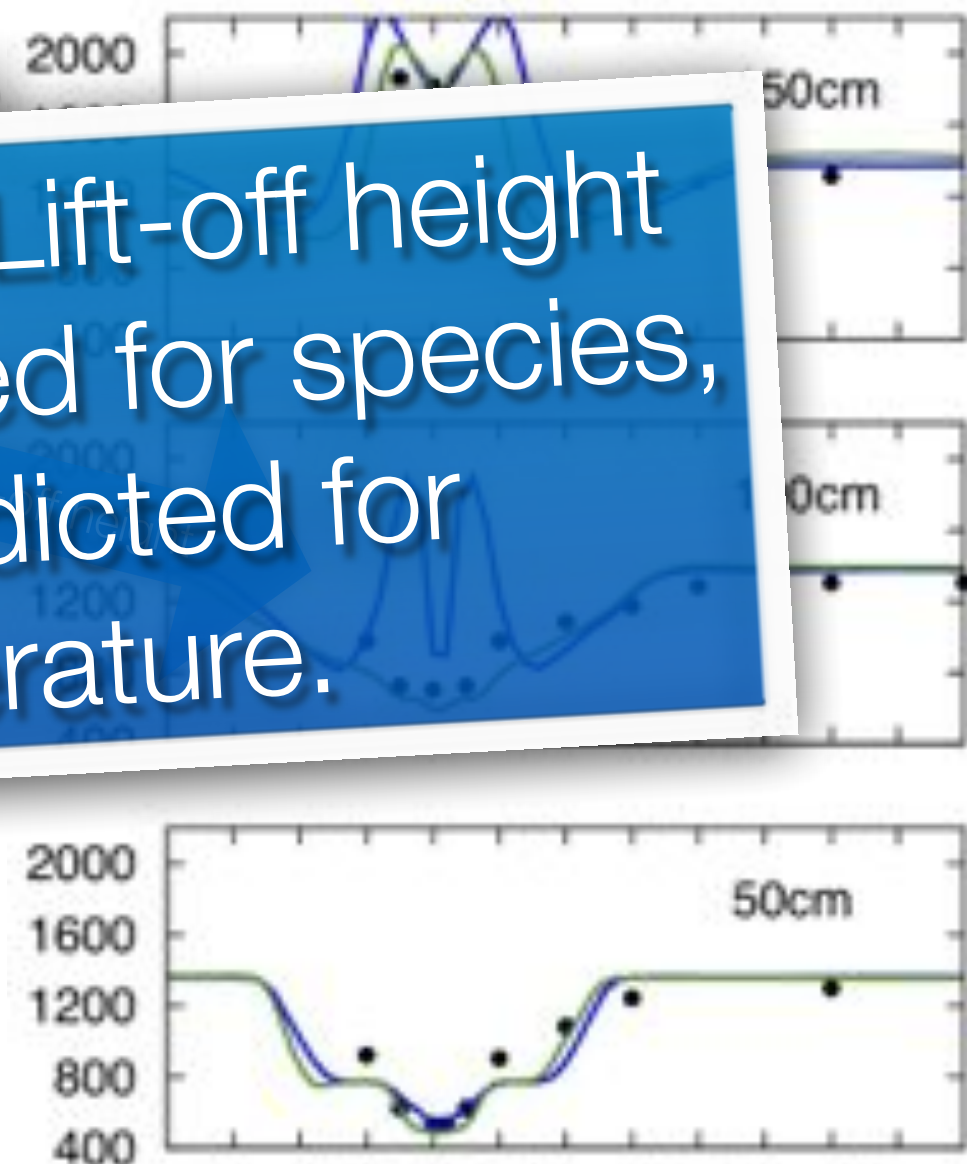


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Mean axial velocity

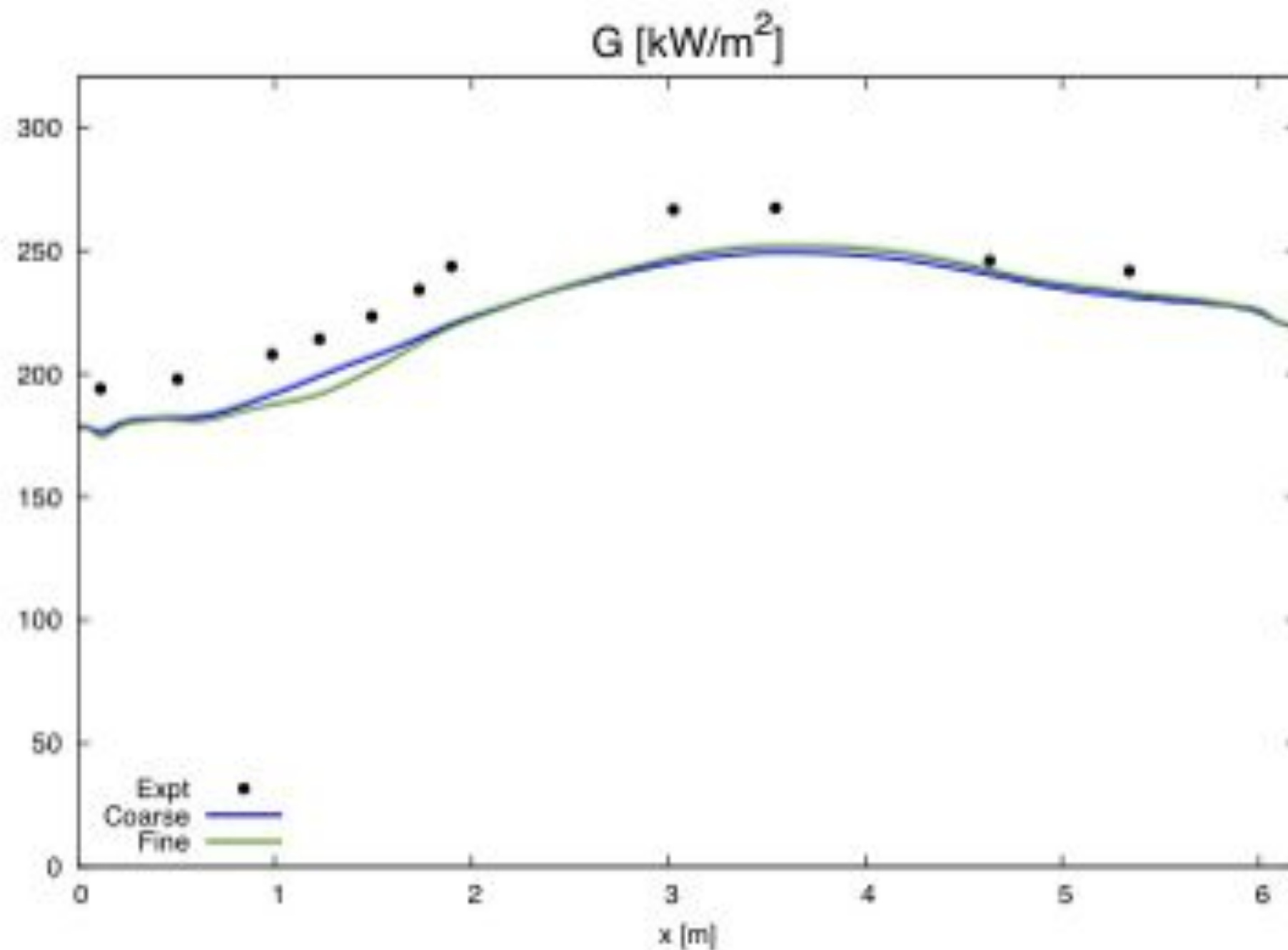


Temperature



Please note: Lift-off height under predicted for species, over-predicted for temperature.

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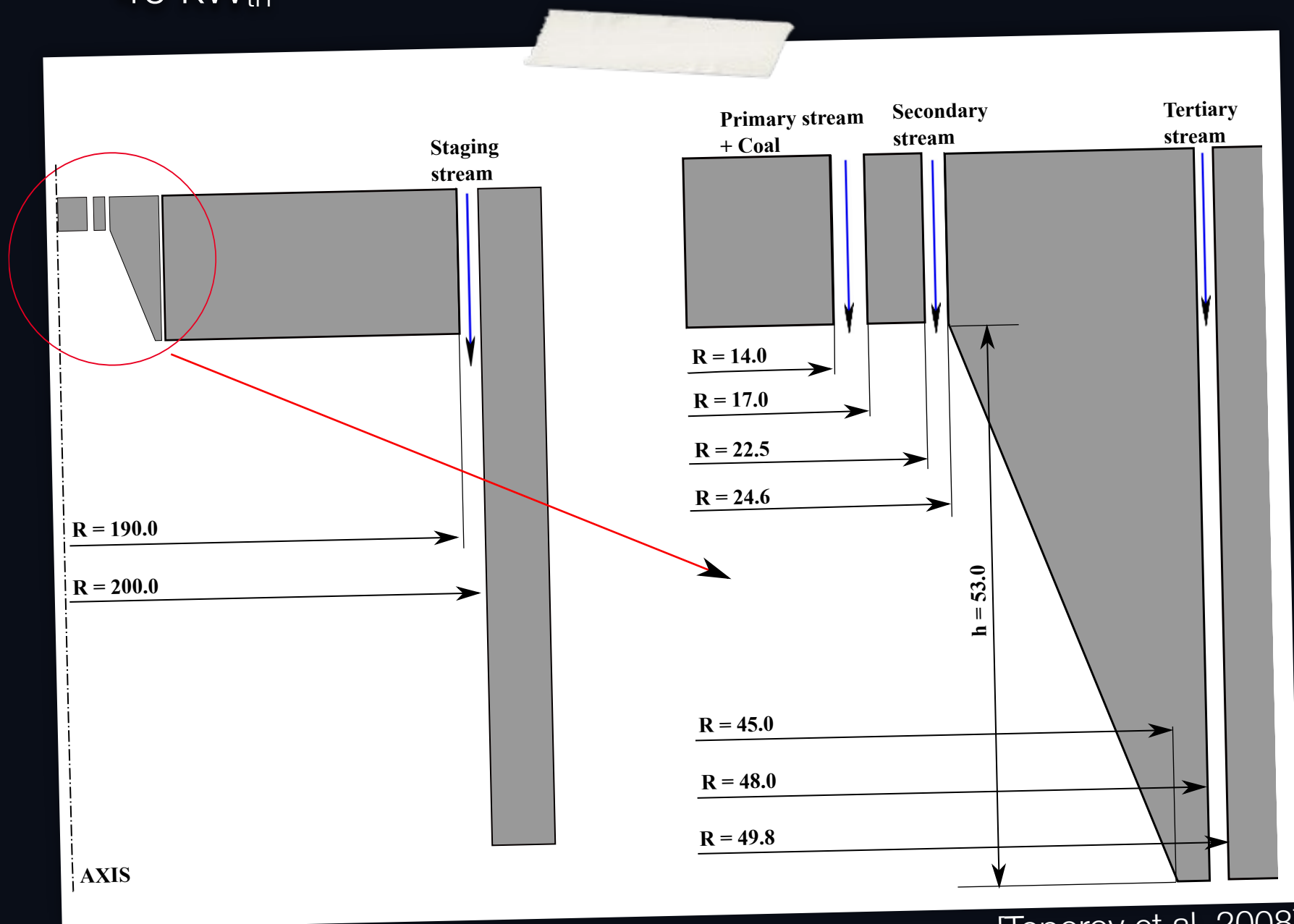


# Aachen OXYCOAL-AC furnace

- Realistic swirl burner
- Oxyfuel
- 40 kW<sub>th</sub>

	kg/h	O	T
Coal feed	6,5	-	-
Primary	17,6	0.19/	40
Secondary	26,6	0.21/0.79	60
Tertiary	1,5	0.21/0.79	60
Staging	54,9	0.21/0.79	900

Proximate Analysis	[wt %]
Moisture	8,4
Ash	4,1
Volatile Matter	46,6
Fixed Carbon	40,9



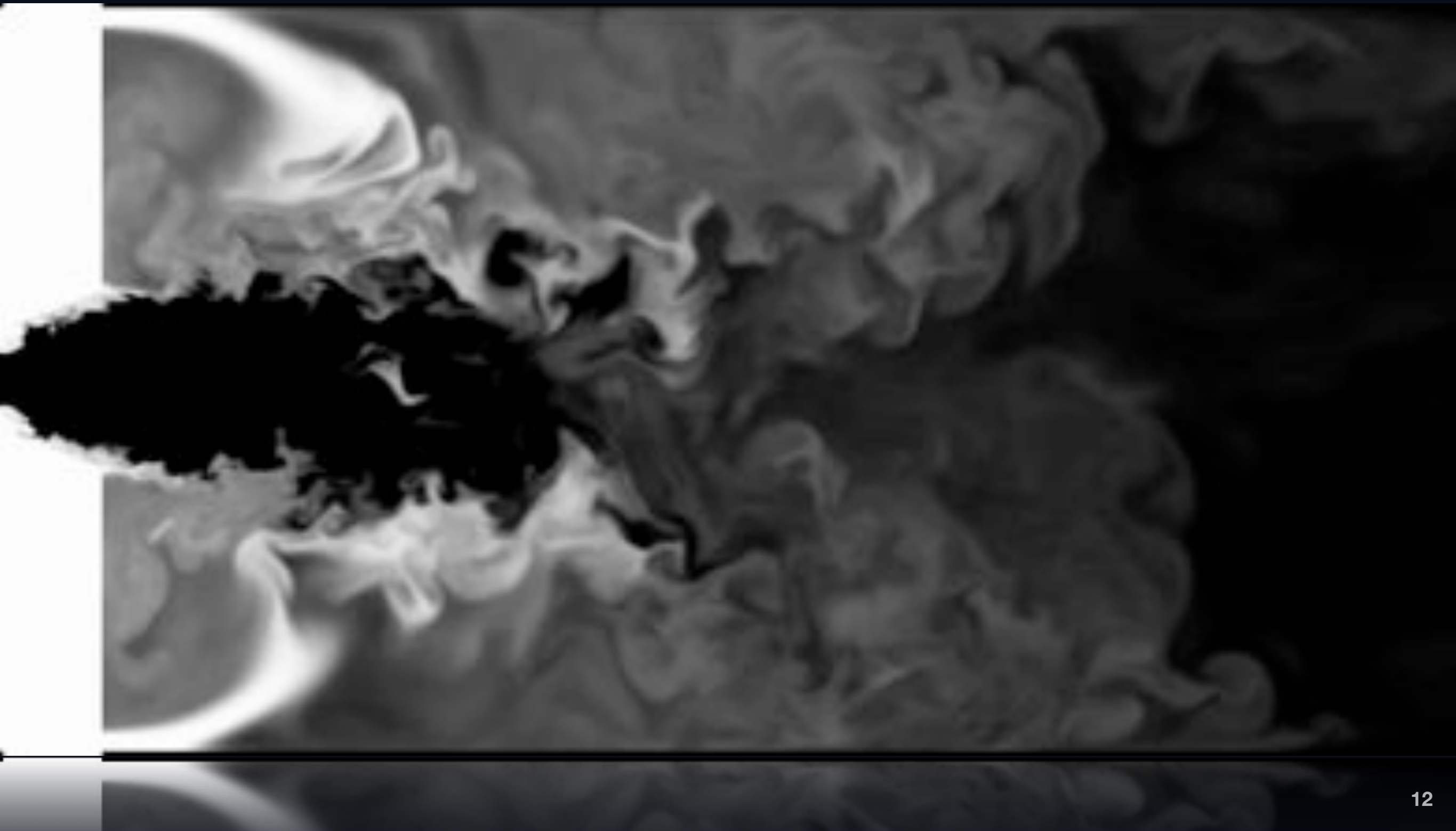
[Toporov et al, 2008]

# Simulation

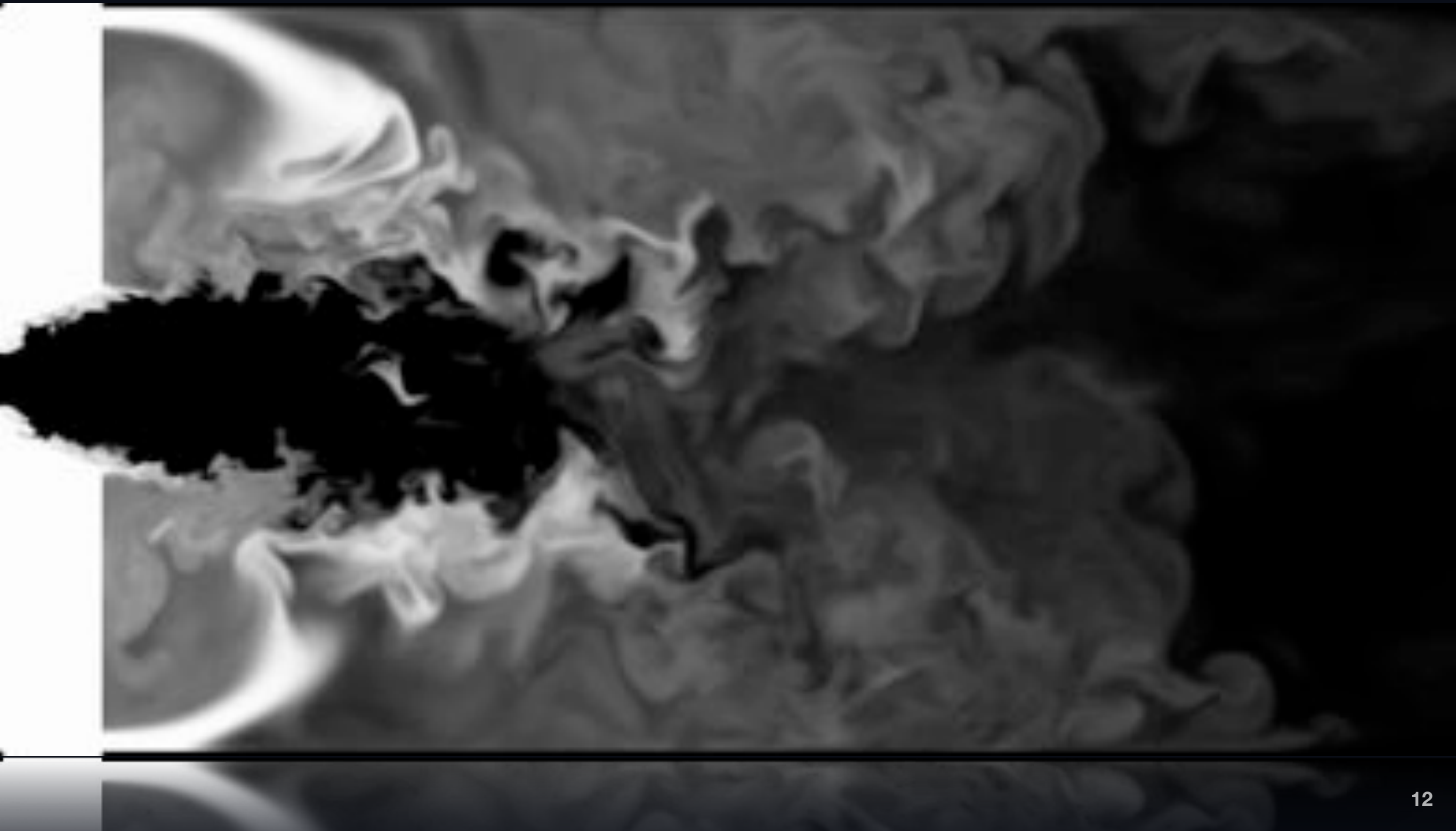
- Cartesian grid: 400 x 400 x 800 mm
- Grid:  $\Delta = 1\text{mm}$ , 128 million cells
- 384 cores, 2 weeks ( $\sim 1000\text{€}$ )
- Ca. 2.5 million numerical particles
- Cray XE6m at Duisburg-Essen & Cluster of Chair

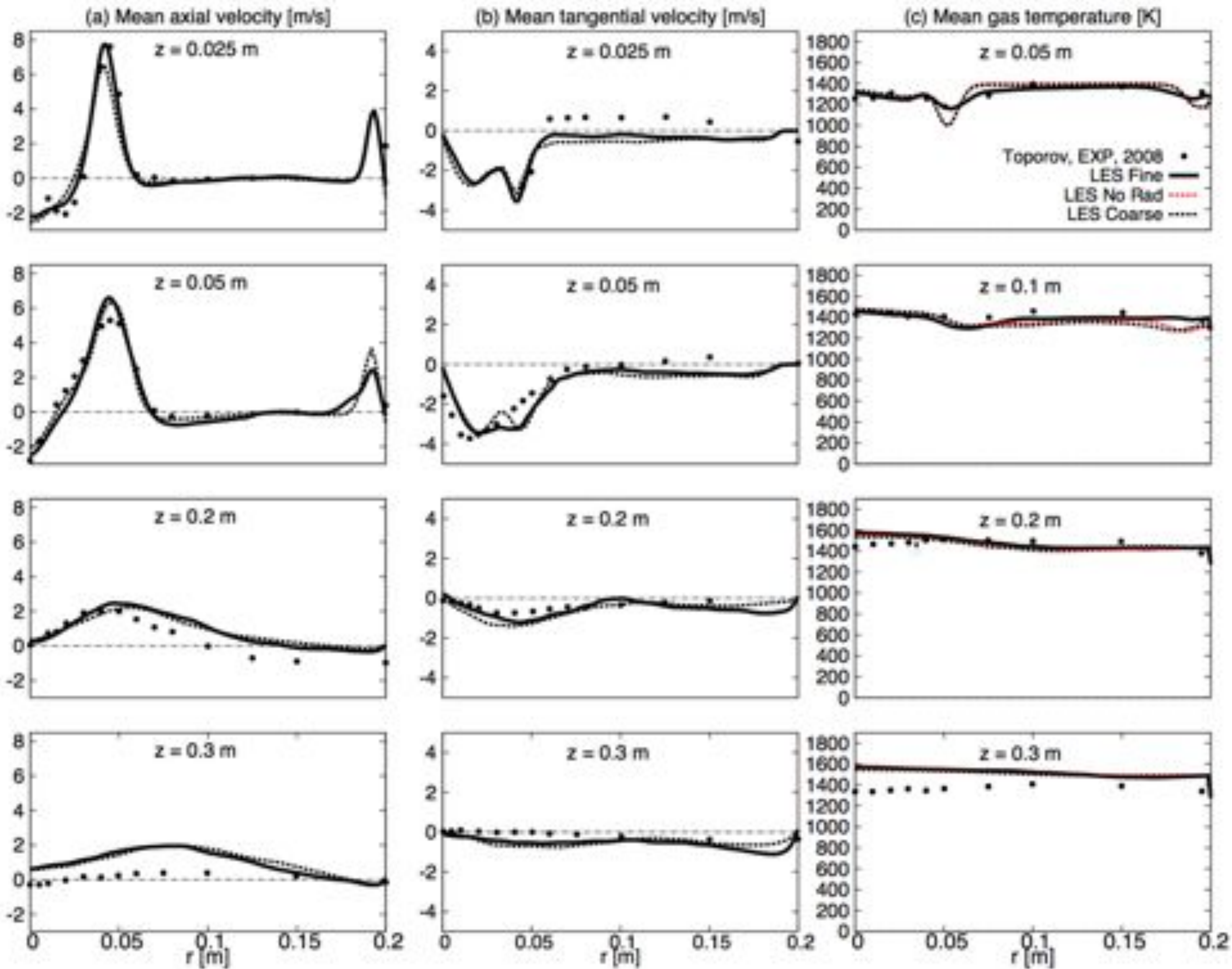


# Mass Fraction Oxygen

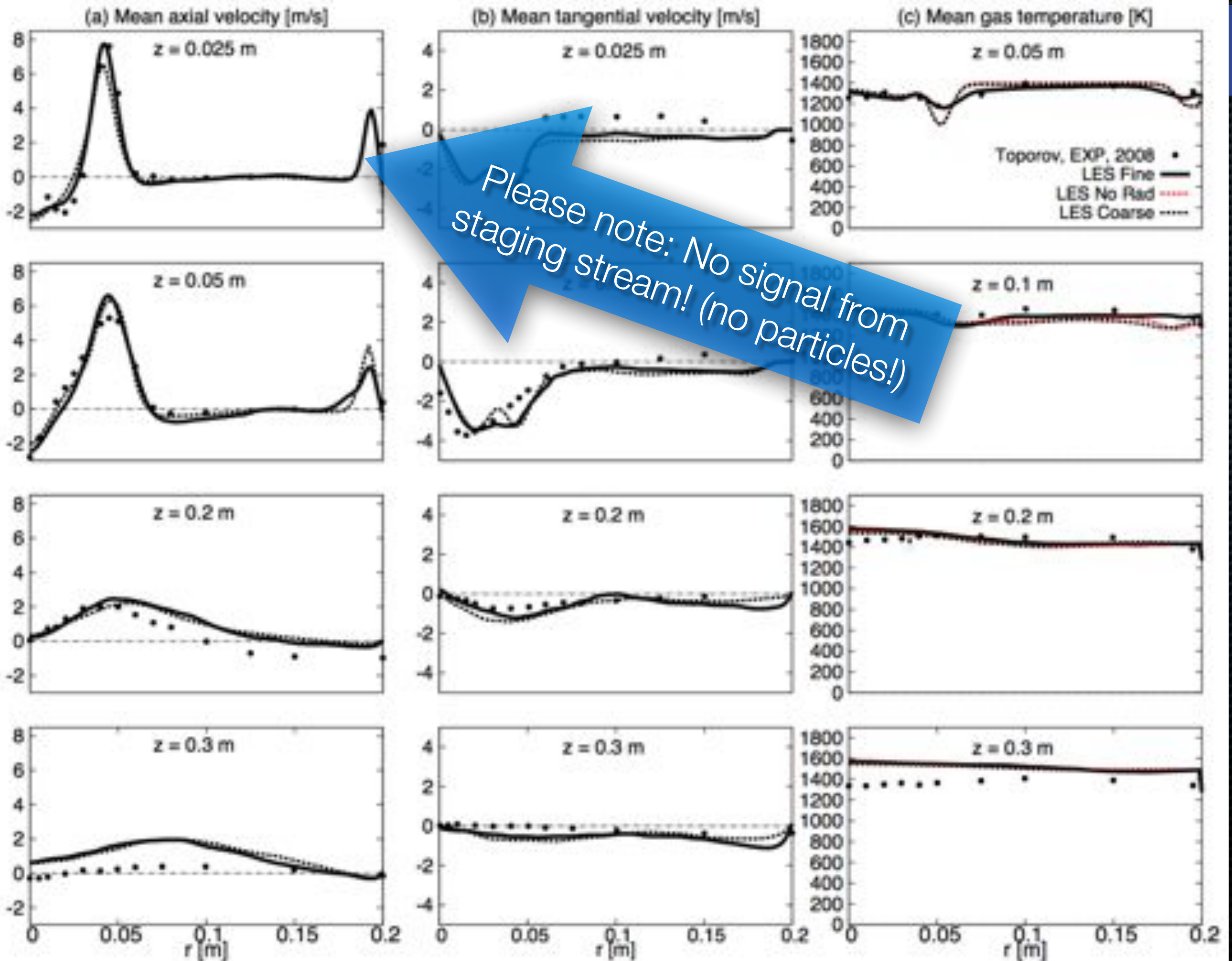


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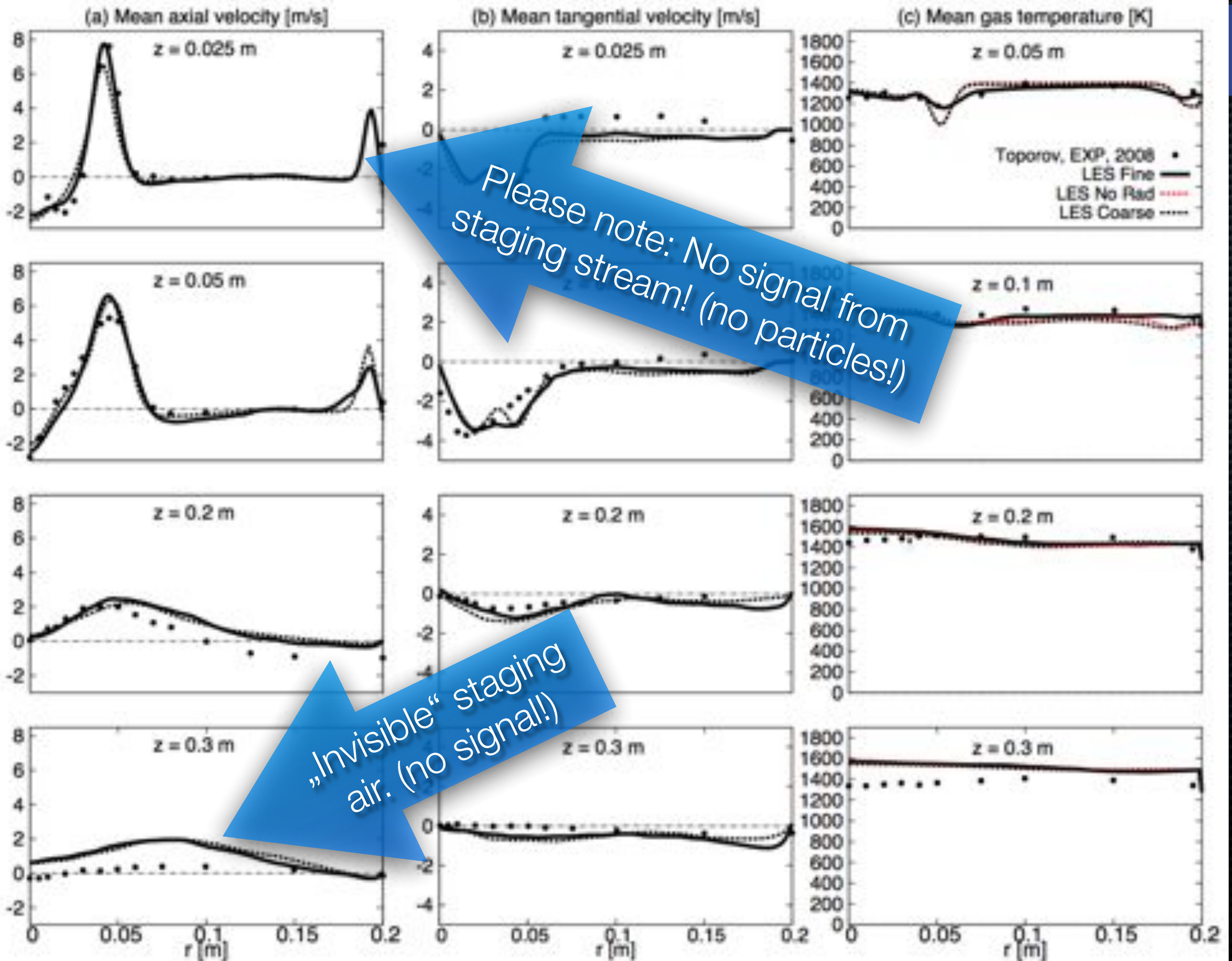


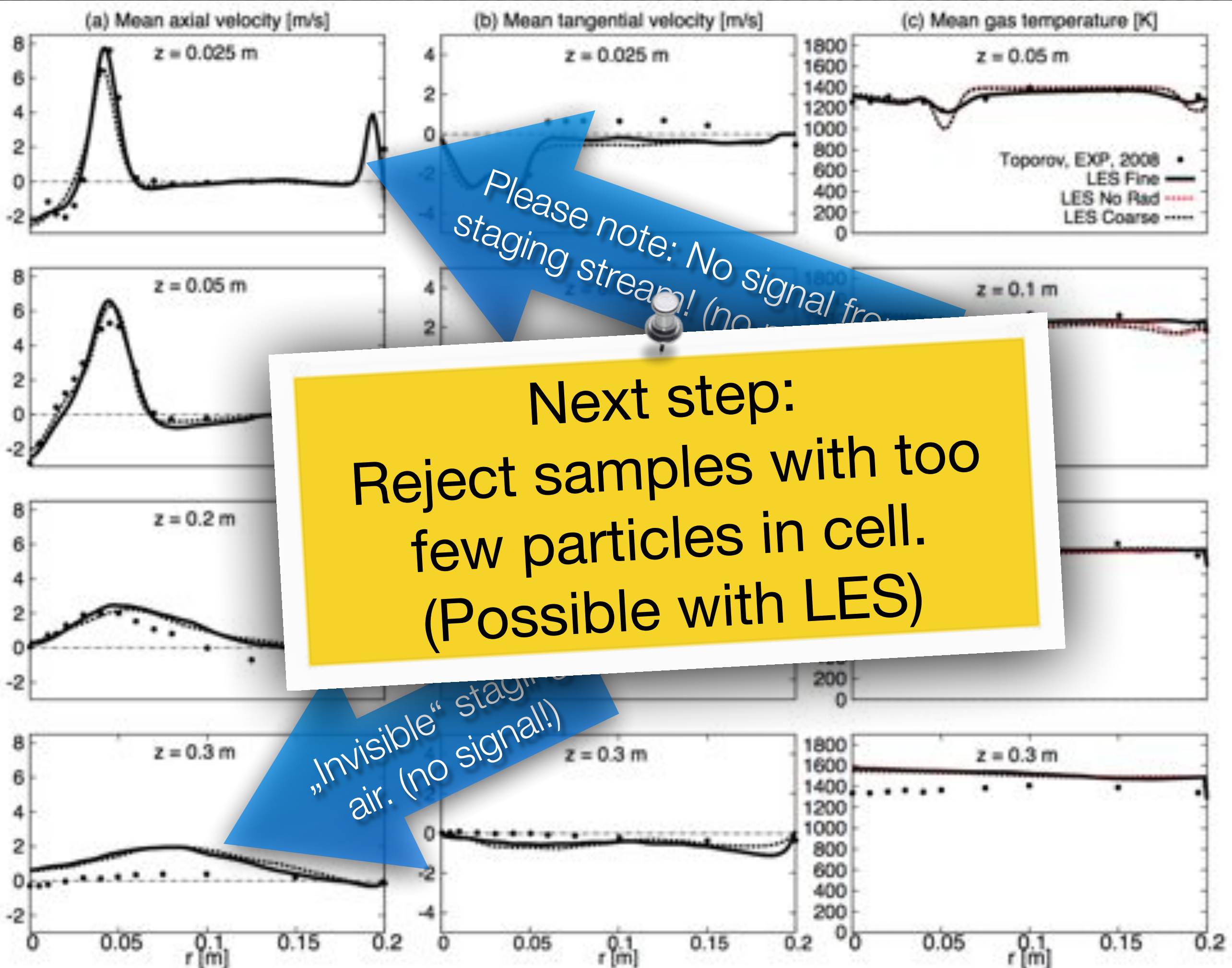






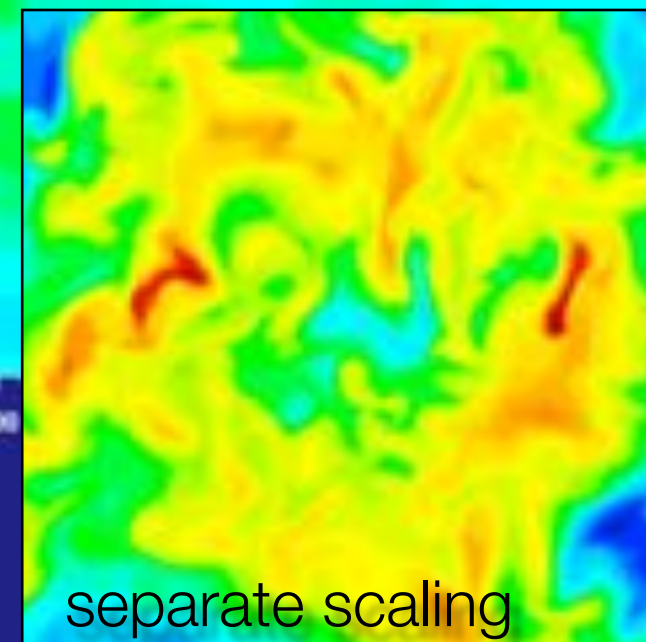
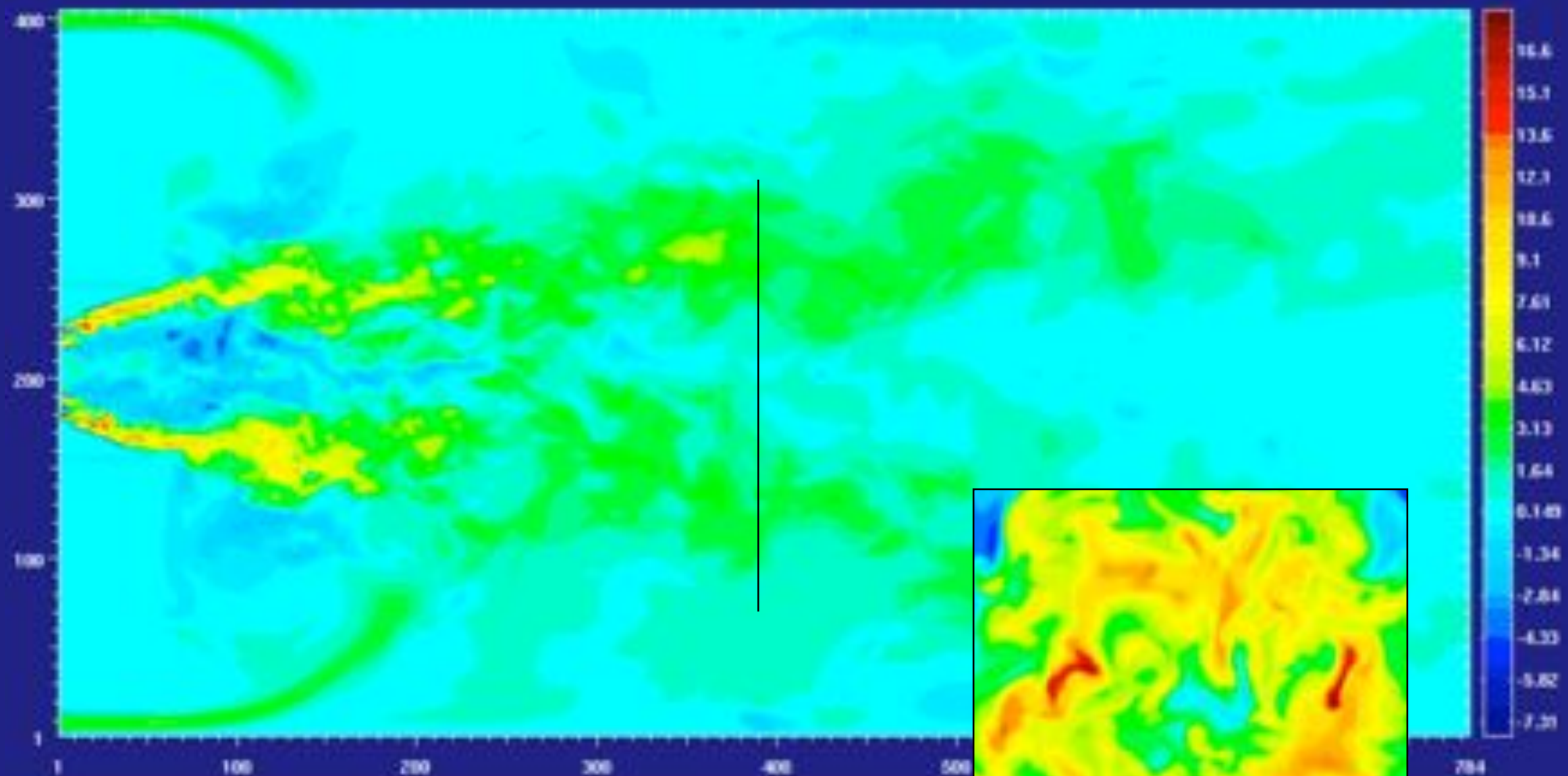




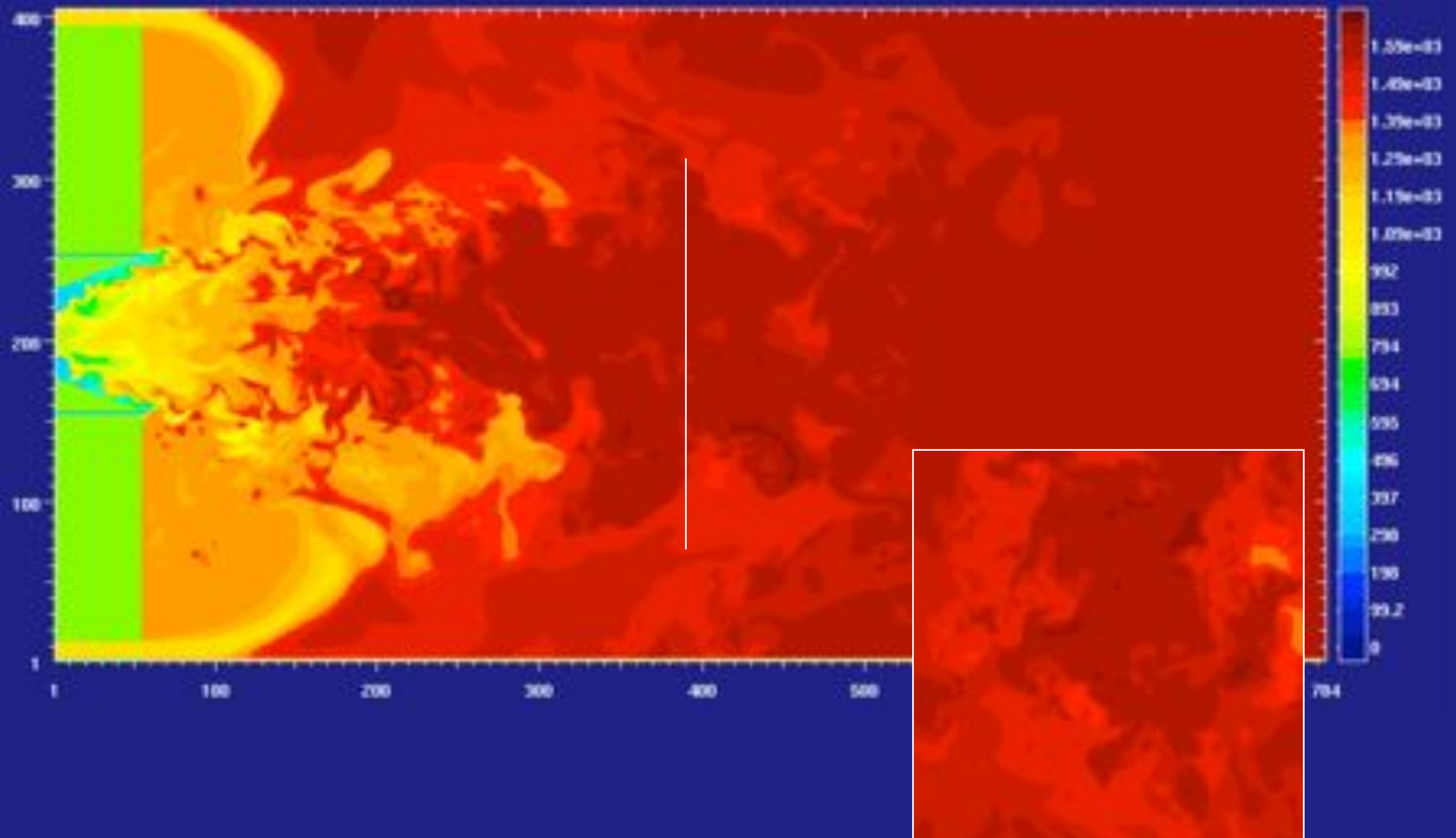




# Axial Velocity

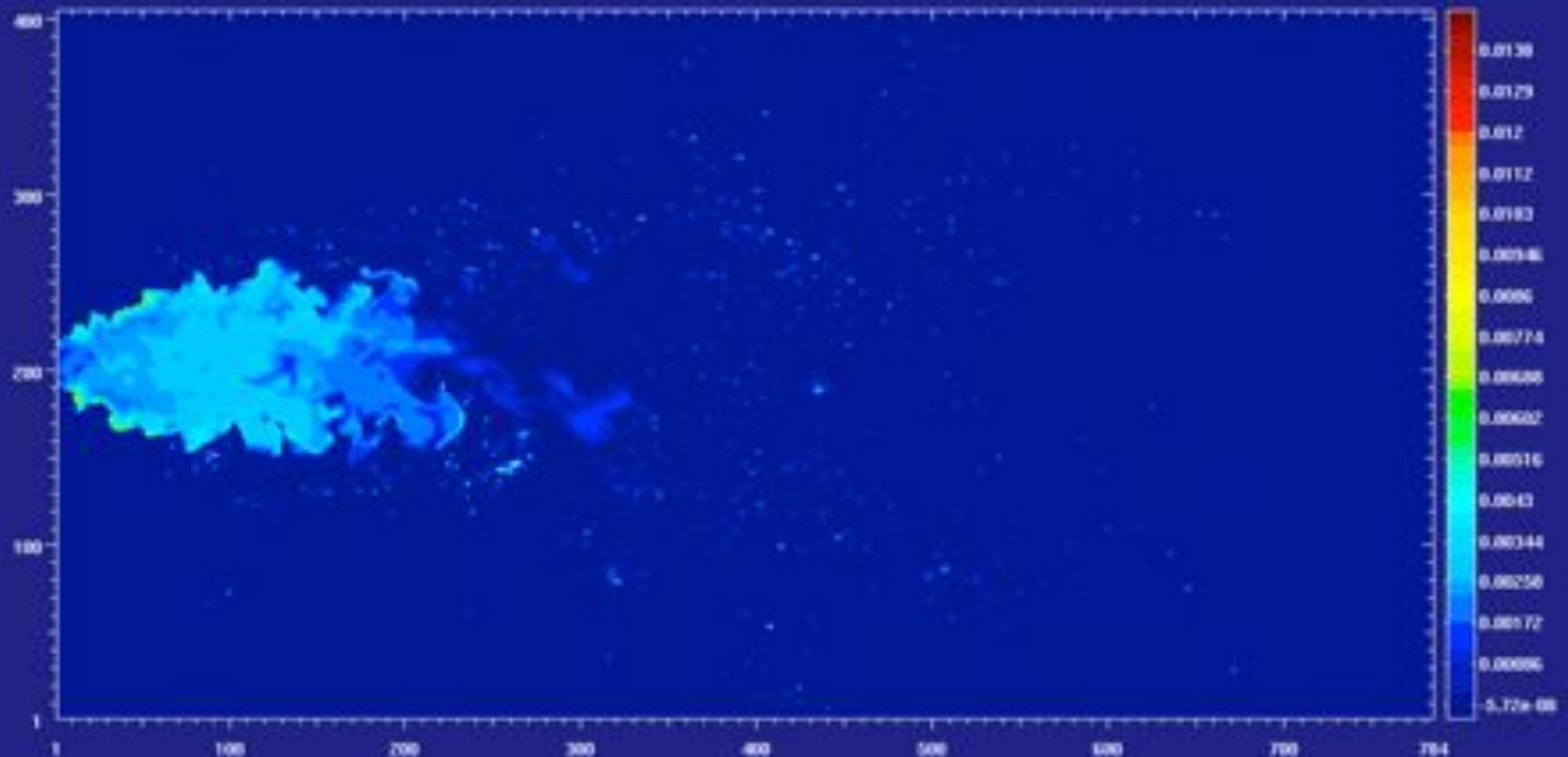


# Gas Temperature

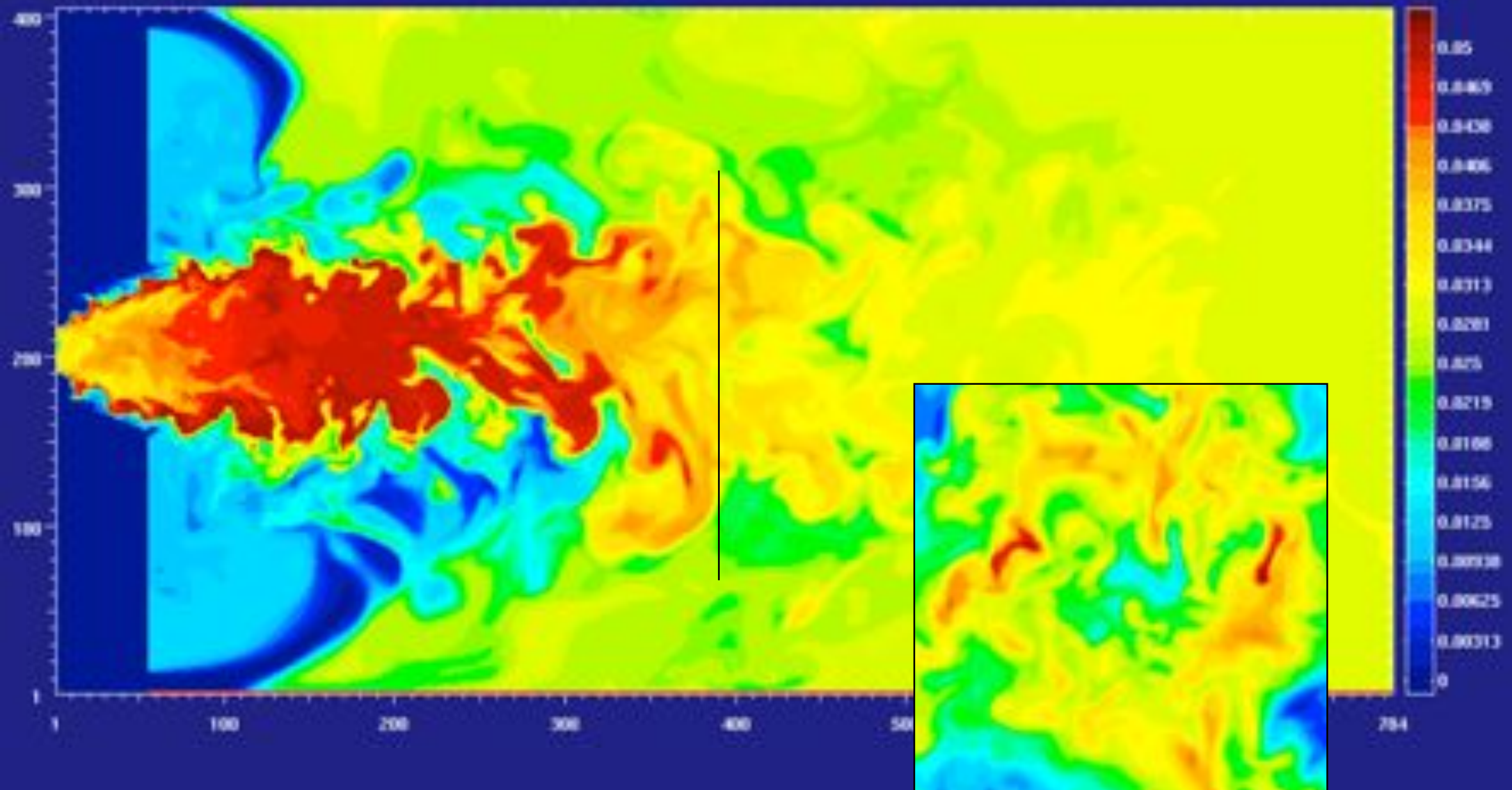




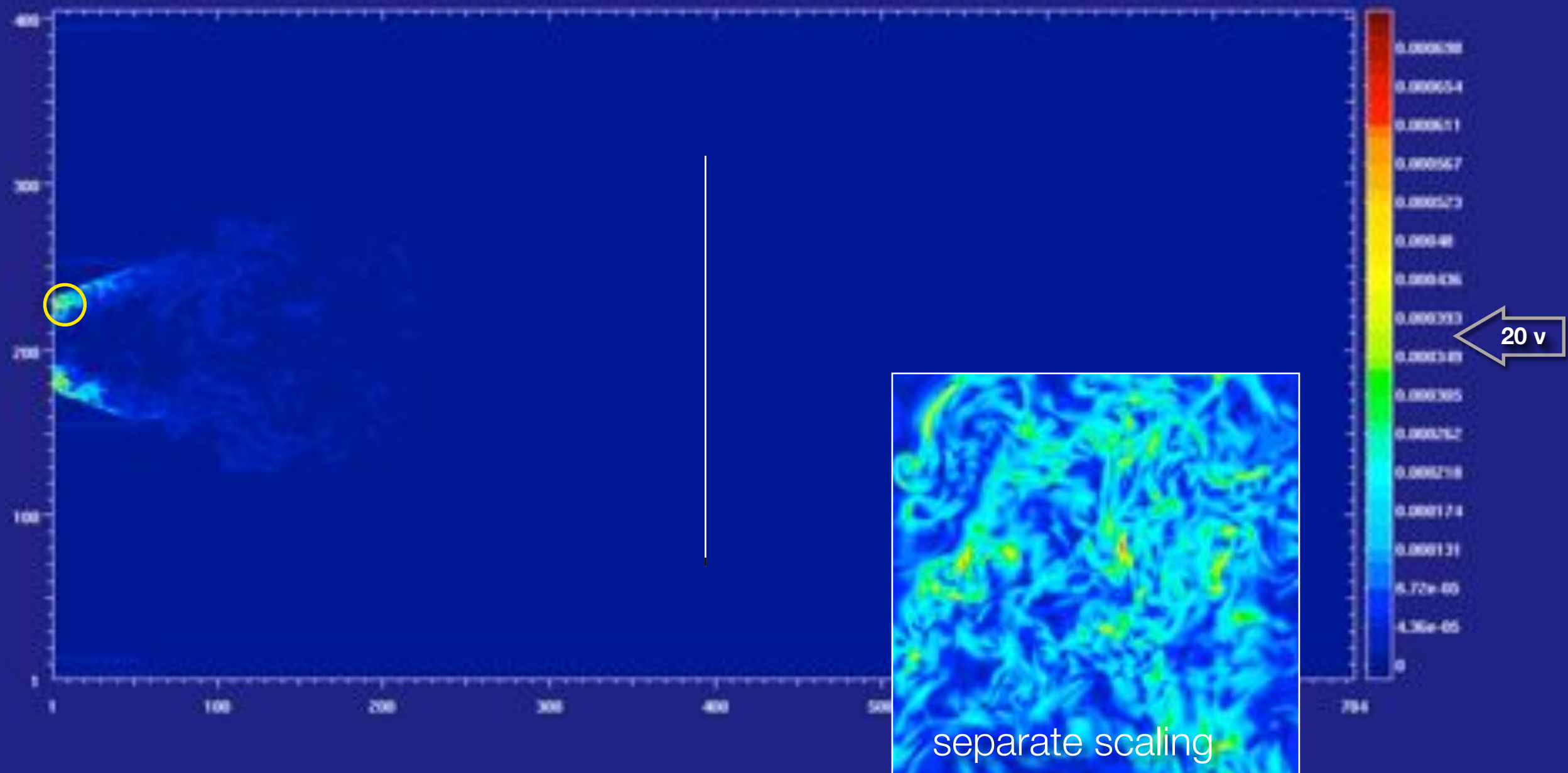
# Mass Fraction CO



# Mass Fraction $\text{H}_2\text{O}$



# Eddy Viscosity





# Symposium 2014

Assessment by a reviewer:

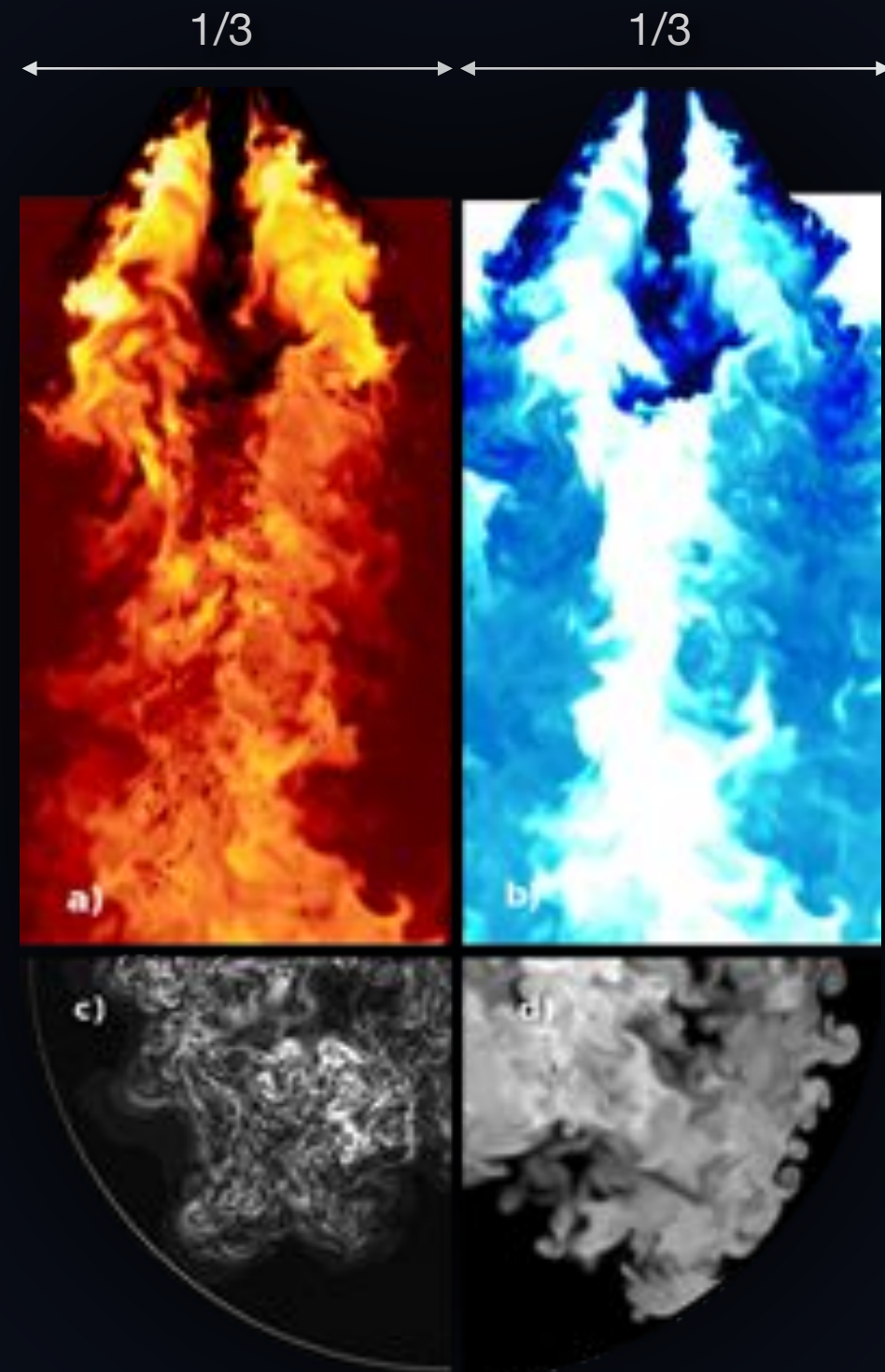
“Oxy-fuel coal combustion systems will not be in operation soon (most probably even never) so the authors should orient their efforts to the air burning of low quality coals...”

separate

# Peak into latest work

- ✦ IST Large Scale Lab Furnace, 100kW,  $D=0.6\text{m}$
- ✦ Work by M. Rabacal, co-supervised by Mario Costa
- ✦ 365 M cells of 1mm
- ✦ HPC: 8000 cores (PRACE, SuperMUC)

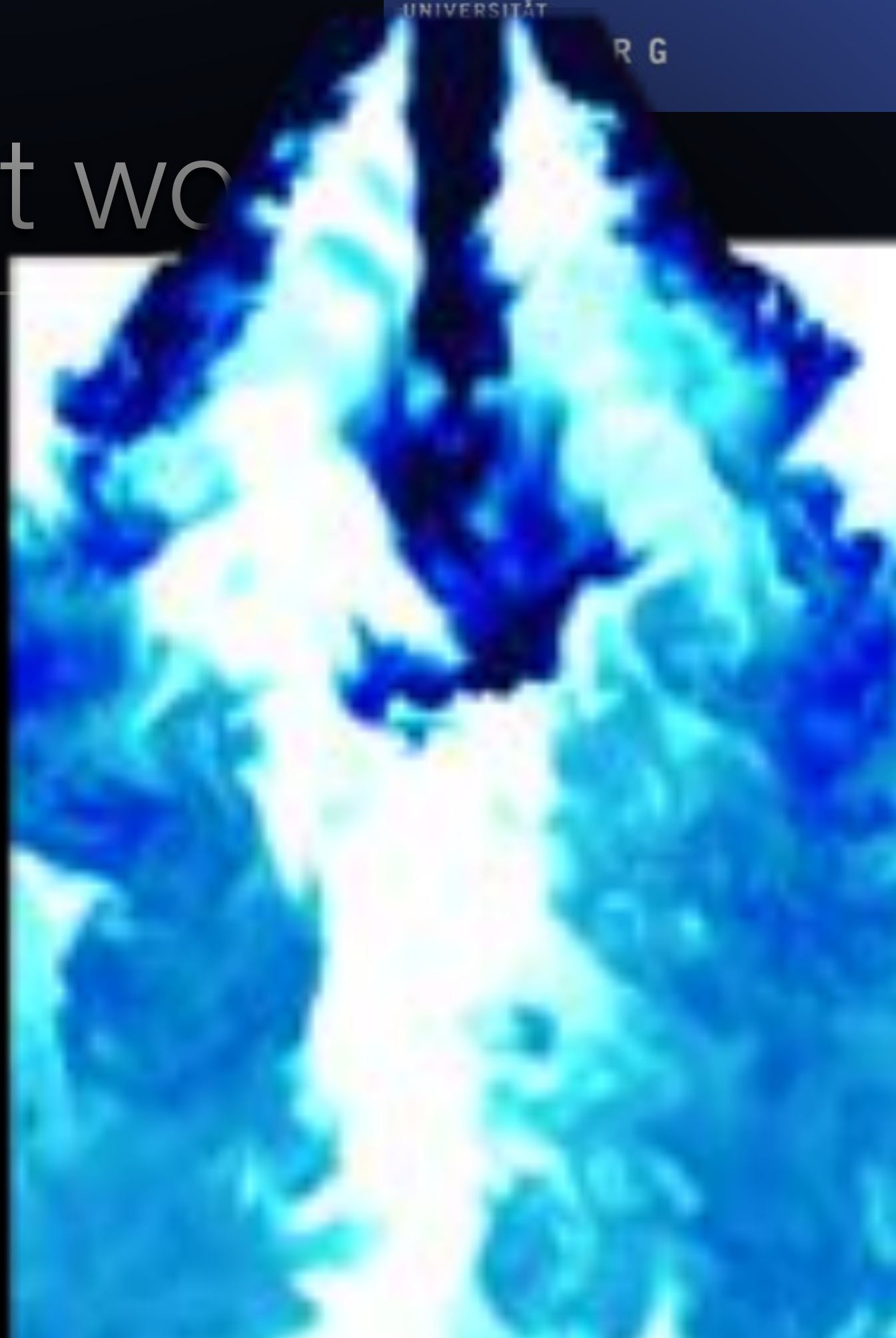
*(accepted)*





P

latest wo





# Summary

- ✦ LES of coal combustion is a reality (new paradigm!)
- ✦ Pilot-scale combustors can be predicted reasonably
- ✦ Now: Time to apply and time to improve sub models
  - ✦ Subgrid modelling
  - ✦ Devolatilisation Modelling
  - ✦ Radiation
- ✦ Gas phase combustion (M. Rieth, Duisburg) (Flamelets, DFG Project with Hasse, Kronenburg)
- ✦ Biomass combustion (M. Rabacal, Duisburg)

# Acknowledgements

EPSRC OxyCAP, EPSRC China

FCT (Portugal)

Center for Computational Sciences and Simulation  
(CCSS) of Duisburg-Essen University

PRACE & SuperMUC

Nguyen, Proch, Rittler, Stein, Pettit, Wysocki, Ma, Rieth

Gibbins, Hasse, Costa

***Thank you for your attention!***