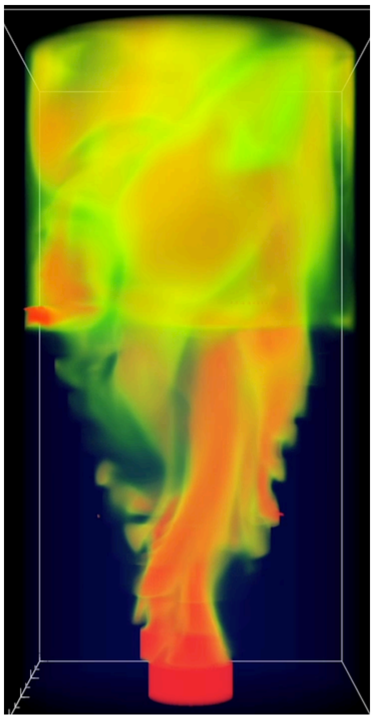
High Resolution Numerical Simulations of Coal Gasifiers Using High Performance Computing



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DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

Presentation Outline

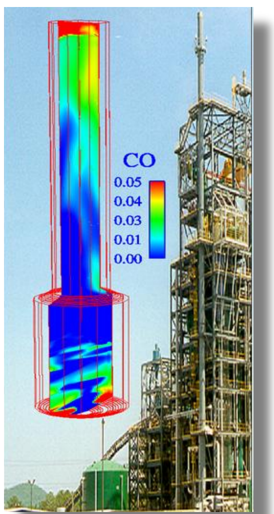
- Motivation for High Resolution Numerical Simulations of Gasifiers Using HPC
- Why Gasifier Simulations Are Compute Intensive?
- Performance Metric
- MFIX & Historical Perspective
- Simulations Conducted with the INCITE Award
- Case B: Nonproprietary Configuration
- Case C: Reduced Configuration
- Conclusions

Motivation

- **High-fidelity gasifier simulations are needed for several reasons:**
  - Better understanding of the governing physics & scientific discovery.
  - Scalability study for new gasifier technology development form lab scale to commercial scale.
  - Optimization for robustness in performance.
  - Trouble shooting operational problems.
- **Strong need for shorter cycle in time-to-market for gasifier technology development and deployment.**
- **Ability to conduct sufficiently accurate and fast gasifier simulations is important for the carbon constrained world.**
- **However, gasifier simulations are inherently compute intensive especially at the commercial scale.**

Challenge: How can we design commercial scale gasifiers for optimized operation?

Use validated computer models for answering scale up questions

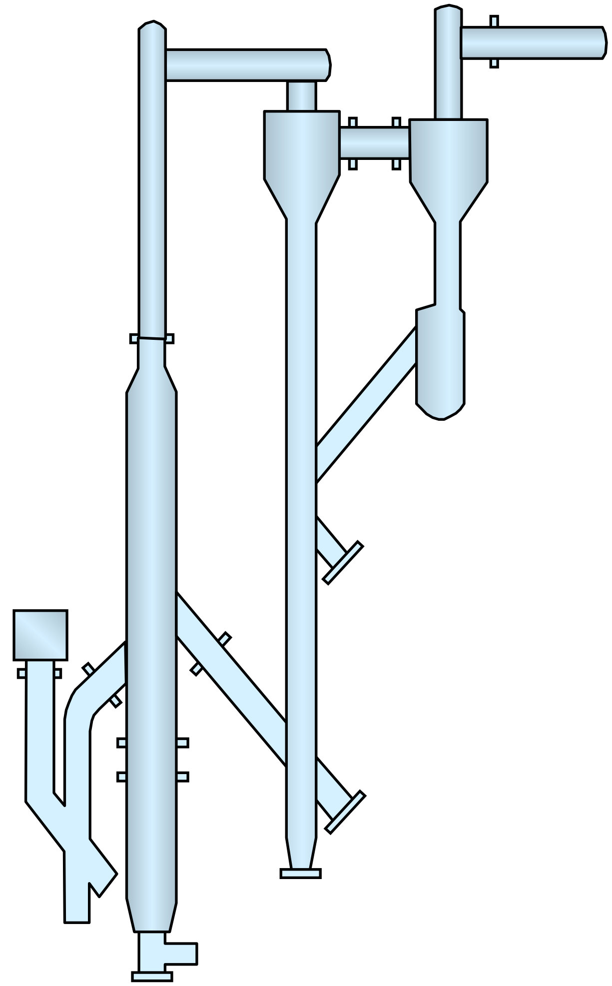


MFIX simulation of pilot scale 13 MW transport gasifier at Wilsonville, AL. Validation of the computer model with prototype system C. Guenther et al (2003)

Parametric Study

- Length/Diameter
- Coal feed rate
- Solids circulation rate
- Recycled syngas
- Coal jet penetration

Coal jet penetration study conducted by NETL is being used by KBR in the design of their commercial scale gasifier.



285 MW Commercial Gasifier

Why Gasifier Simulations Are Computationally Intensive?

- **Long duration computation needed:**
  - Typical simulated time duration is 10 to 15 sec
- **Adaptive and small time-steps are required:**
  - Average time-step size ranging from 10^{-5} to 10^{-4} sec
- **Strong non-linearity stems from the complex interactions between the gas and solid phases, the chemical species reactions, and heat transfer:**
  - Several non-linear iterations required per time-step

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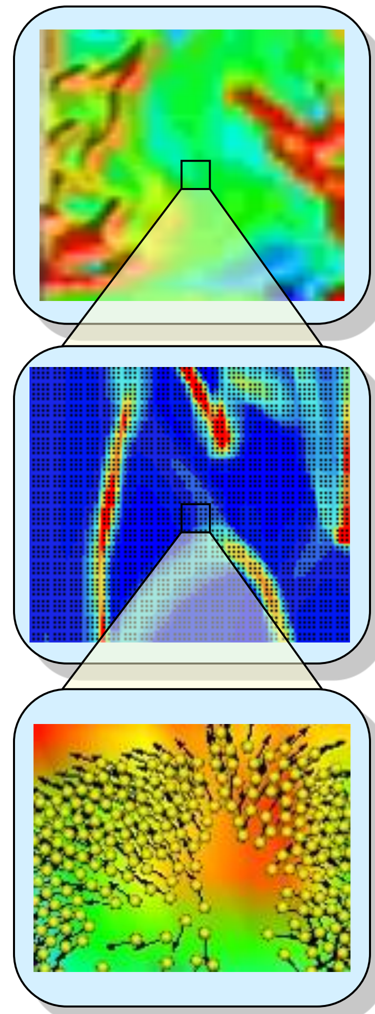
Why Gasifier Simulations Are Computationally Intensive? (cont'd)

- **Numerical grid resolution requirement for grid independency is significant:**
  - For a typical industrial scale riser of 1 m diameter & 30 m height with coal particles of 100 microns (averaged):
    - 24 billion cell grid resolution needed if uniformly 1 mm resolution to be achieved.
    - Simulating at this resolution is beyond the current and near future computational capability.
    - Achieving 1 mm resolution **only in certain regions of interest** has become feasible with the advances in high performance computing in the last decade.



Levels of averaging: discrete particles to continuum to filtered-continuum models

Performance Metric: Simulated time per wall-clock time

- **Inherently transient nature of the process requires long duration of simulation before any useful insight can be gained**
  - For 10M cell resolution, approximately 3M hrs on jaguar(XT4)@NCCS used to generate 12 sec duration simulation in 2008 for single design configuration.
- **Target (2006 NETL Multiphase Roadmap): Overnight turnaround**

  (i.e., ~ 10 – 12 hrs)
- To achieve the target it was necessary to improve performance of the CFD code for today's modern many-core heterogeneous HPC platforms.

MFIX, Open Source Multiphase Flow Code

Mass conservation for phase m (m=g for gas and s for solids)

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{N_m} R_{ml}$$

Momentum conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \overline{\overline{S}}_m + \varepsilon_m \rho_m \vec{g} + \sum_n \vec{I}_{mn}$$

Granular energy conservation (m ≠ g)

$$\frac{3}{2}\varepsilon_m \rho_m \left(\frac{\partial \Theta_m}{\partial t} + \vec{v}_m \cdot \nabla \Theta_m \right) = \nabla \cdot \vec{q}_{\Theta_m} + \overline{\overline{S}}_m : \nabla \vec{v}_m - \varepsilon_m \rho_m J_m + \prod_{\Theta_m}$$

Energy conservation

$$\varepsilon_m \rho_m C_{pm} \left(\frac{\partial T_m}{\partial t} + \vec{v}_m \cdot \nabla T_m \right) = -\nabla \cdot \vec{q}_m + \sum_n \gamma_{mn} (T_n - T_m) - \Delta H_{rm}$$

Species mass conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{ml}) + \nabla \cdot (\varepsilon_m \rho_m X_{ml} \vec{v}_m) = R_{ml}$$

http://mfix.netl.doe.gov

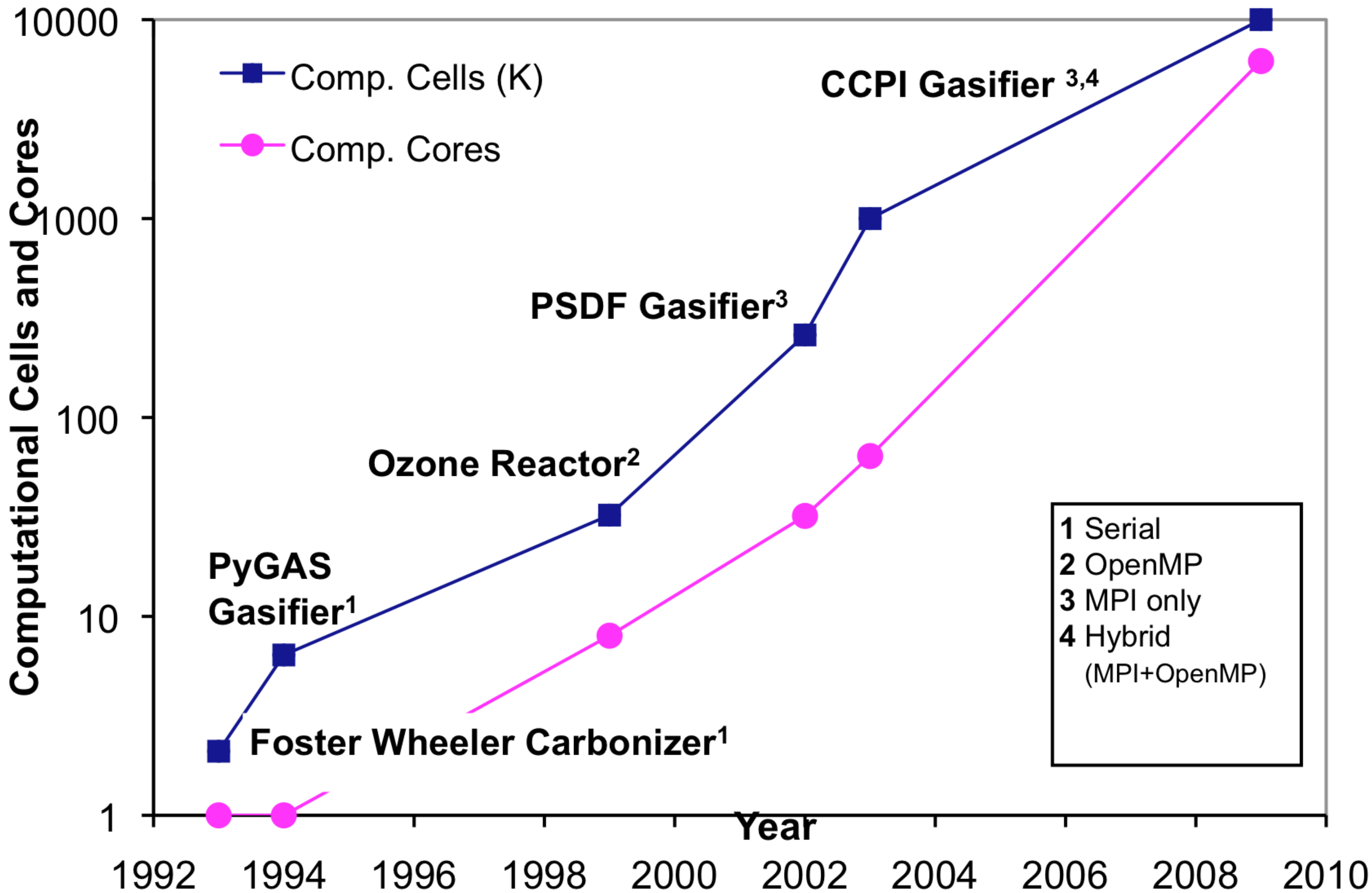
R&D100 Award 2007

Excellence in Technology Transfer Award 2008 for C3M

Tech-Transfer Award 2006

- Syamlal et al. "MFIX Documentation, Theory Guide," DOE/METC-94/1004, NTIS/DE94000087 (1993)
- Benyahia et al. "Summary of MFIX Equations 2005-4", From URL http://www.mfix.org/documentation/MfixEquations2005-4-3.pdf, July 2007.

Historical Perspective: Reactor simulations with MFIX over the years



Performance Improvements

– Extensive profiling of MFIX with TAU on various HPC platforms to understand bottlenecks on modern systems.

– Multiple improvement phases were incorporated based on profiling results & are still under progress:

- **Phase I**: Choice of compiler flags and MPI tuning parameters
- **Phase II**: Reduction of MPI collective calls in linear equation solver and compile with PathScale instead of PGI.
- **Phase III**: Hybrid mode operation of MFIX to take advantage of multi-core platforms with MPI and OpenMP.
- **Phase IV:** Integration of a standard high level I/O library to address I/O bottlenecks (netCDF).
- Phase V: Integration with highly scalable and tuned solver library such as Trilinos [under progress – preliminary version available as of Feb'10].

INCITE Award

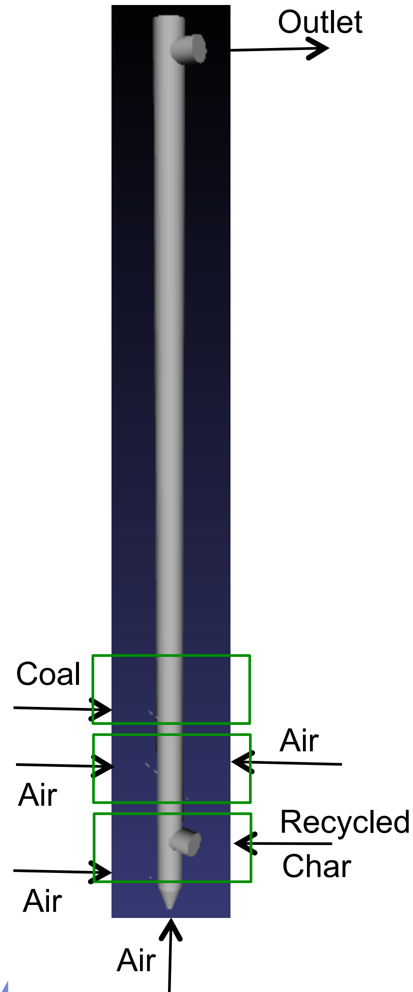
- A total of 22M CPU hours were awarded to NETL by the **Innovative and Novel Computational Impact on Theory and Experiment (INCITE)** program of U.S. Dept. of Energy between 2008-2010.
- **Objective:** To conduct high resolution simulations to provide a detailed flow map of a commercial scale gasifier and provide design feedback to our industrial collaborators.
- **First-of-its-kind MFIX gasifier simulations for two commercial scale and one reduced configurations were completed.**

Simulations Performed with INCITE Award

Case	Case Description	Grid Resolution	Simulated Time (s)	Comp. Cost (CPU hrs /1s simulated time)
A	Proprietary Gasifier Configuration	10M cells	40	L: ~165,000
B	Non-proprietary Configuration	9.8M cells (40x4092x60)	22	L: ~148,600
C	Reduced Configuration	(1) 2.4M cells	10	L: ~12,200 H: ~42,900
		(2) 0.7M cells	10	L: ~7,800 H: ~11,000
		(3) 0.35M cells	10	L: ~7,400 H: ~1,950

All simulations performed on jaguar (Cray XT5) at Oak Ridge National Laboratory (ORNL)
Jobs automatically resubmitted at the end of 12hr batch execution session.
Typically high resolution jobs were executed on 6192 cores (1032 MPI + 5160 OpenMP)

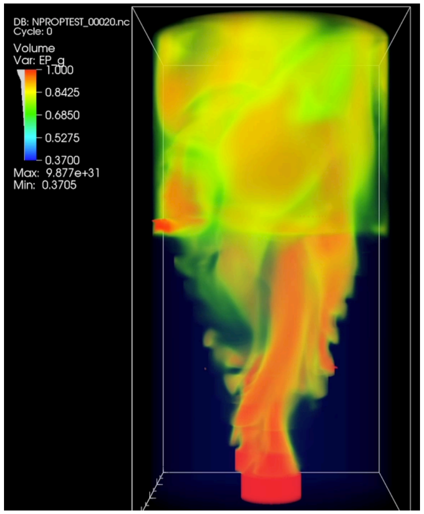
Case B: Nonproprietary Gasifier Configuration

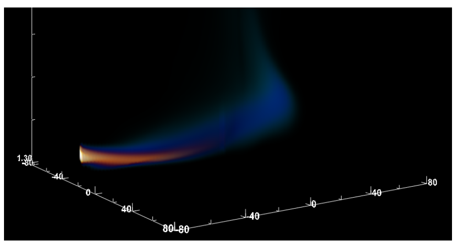


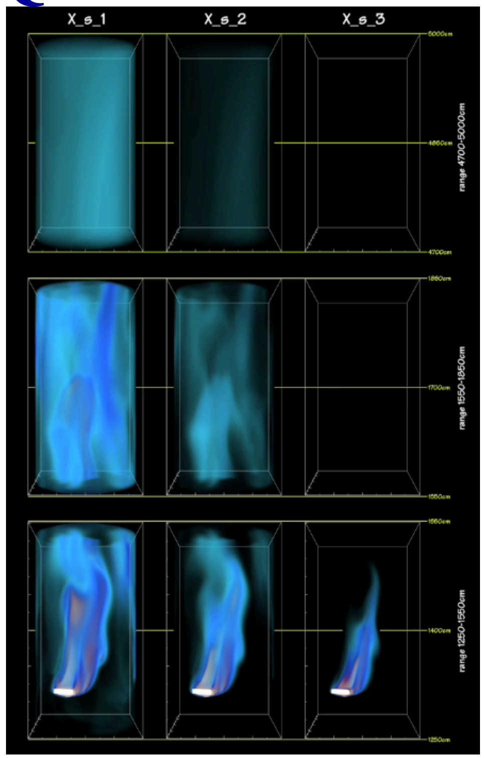
- Geometric configuration : 50m height and 0.8m radius
- Grid resolution : 40 x 4092 x 60 = 9.8 M cells
- Non-uniform grid spacing along the height of the gasifier to achieve 1mm resolution for certain regions.

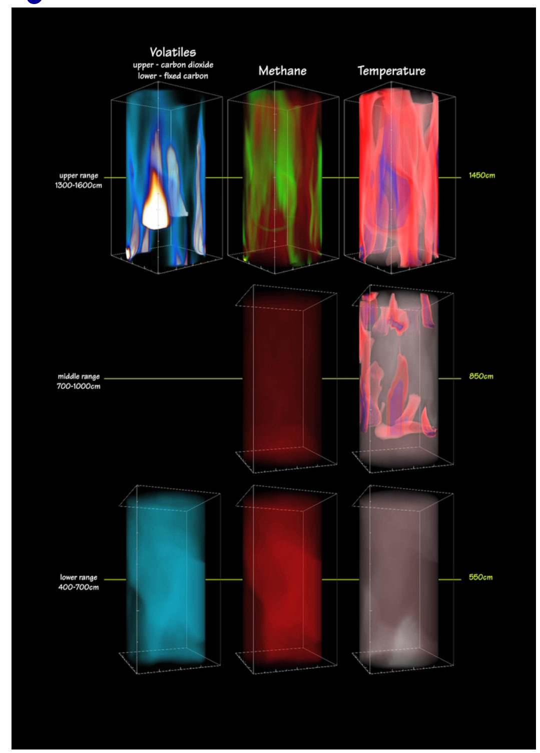
- Eulerian-Eulerian simulation with chemically reacting species transport resolved:
    - 8 Gas phase species (e.g. 0_2, CO, CO_2, CH_4, H_2, H_2O, etc.)
    - 8 Solid phase species (e.g. FC, VM, Moisture, Ash, etc.)
- Coal gasification modeling performed with 2008 Federal Laboratory Consortium (FLC) Award winning Carbonaceous Chemistry for Computational Modeling (C3M) implemented in MFIX
- 2010 version of C3M includes coal GUI interface (URS-Phil Nicoletti) with PC Coal Lab & development of soot chemistry (WVU-Dr. Turton & Kiran Chaudhari)

Preliminary Post-processing of Case B: Nonproprietary Gasifier Configuration for Qualitative Analysis

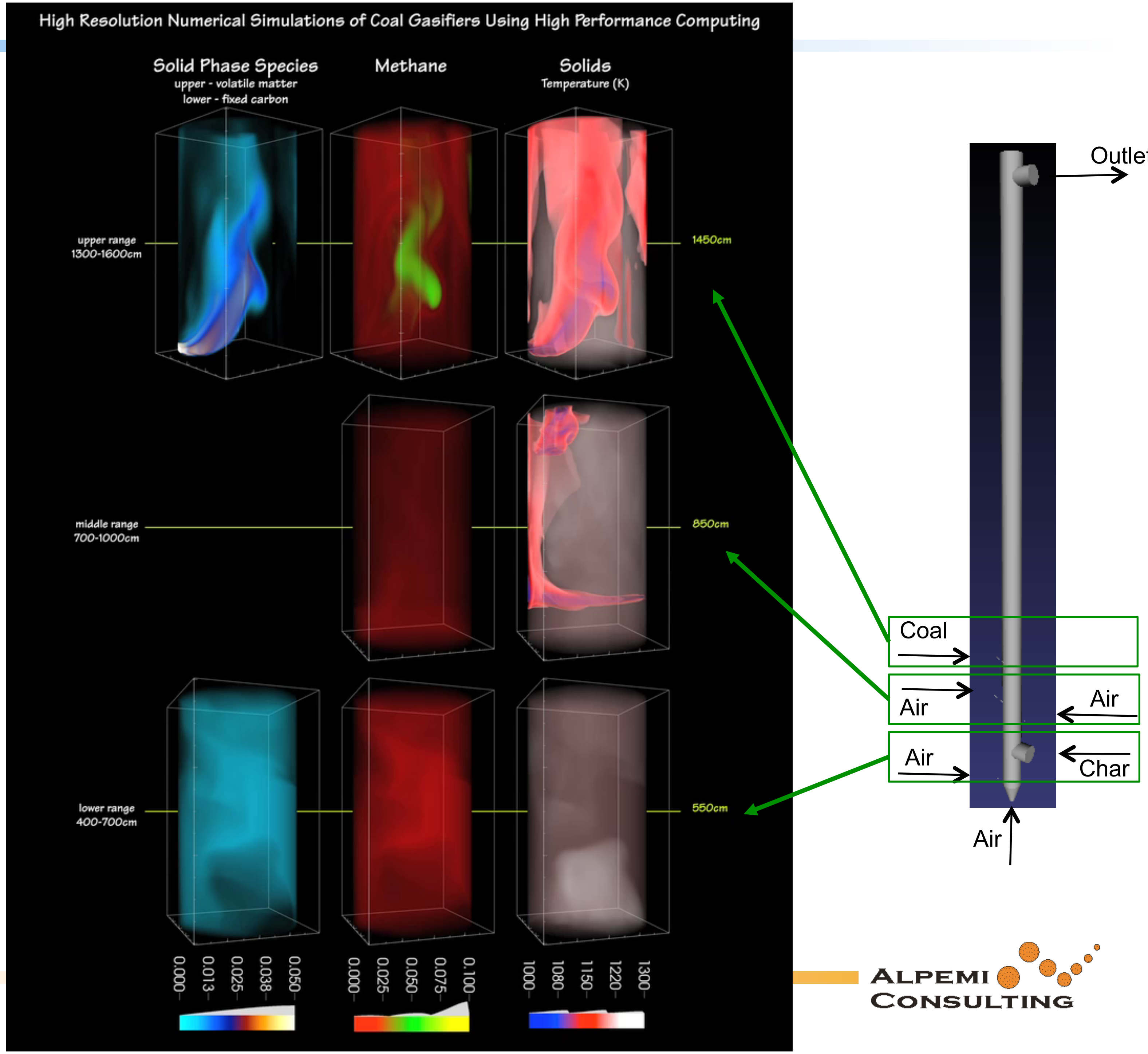








- **Approximately 1 TB data was post-processed, reduced and converted into netCDF.**
- **Visualizations were ray casting based volume rendering.**
- **VisIt visualization package was used in client-server mode:**
  - 16 to 32 processors of visualization cluster@ORNL were employed in volume rendering to compute and generate each single frame and a client desktop system displayed the results.



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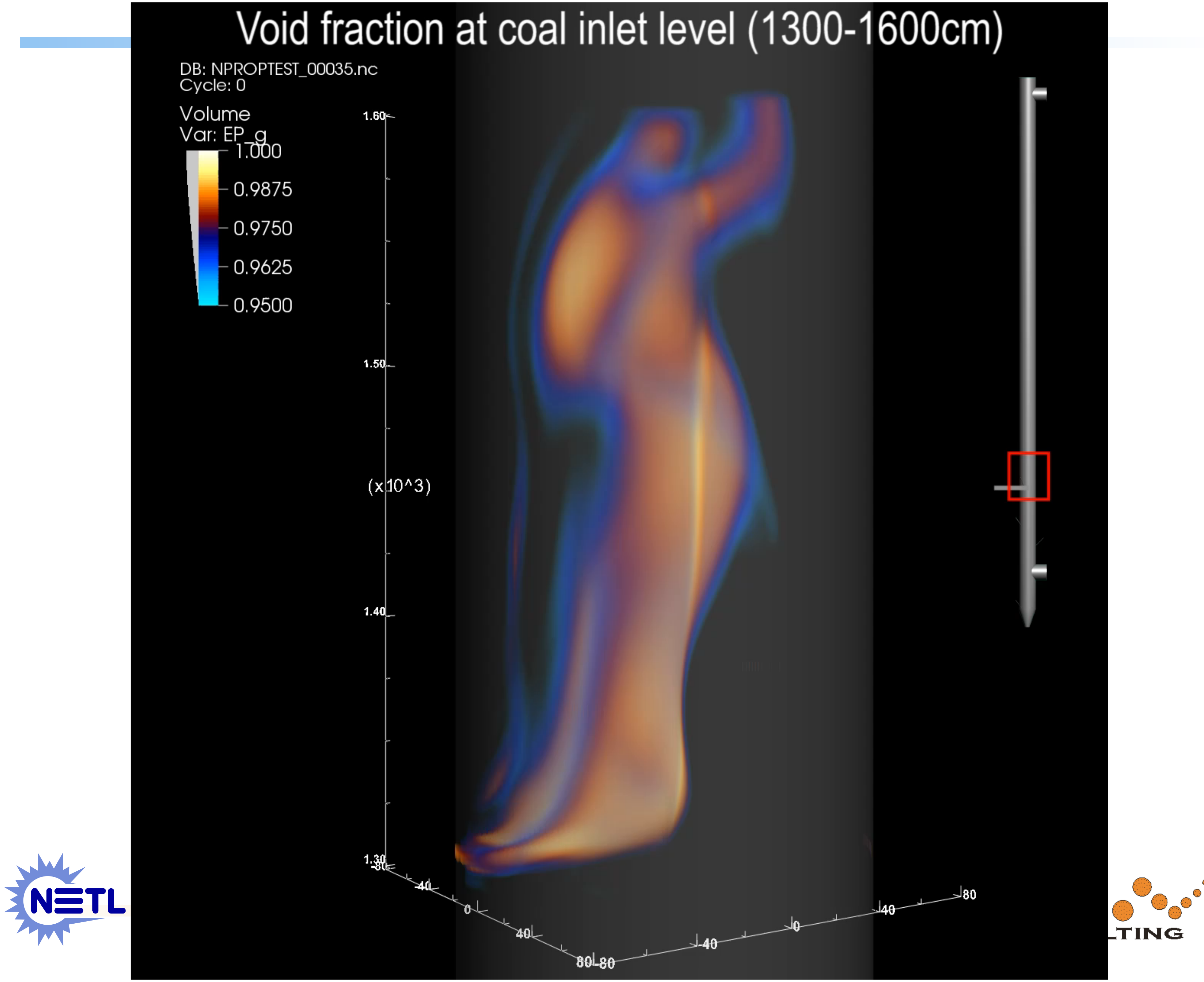
Void fraction at coal inlet level (1300-1600cm)
DB: NPROPTEST_00035.nc
Cycle: 0
Volume
Var: EP_g
1.000
0.9875
0.9750
0.9625
0.9500
1.60
1.50
(x10^3)
1.40
1.30
-80
-40
0
40
80
-80
-40
0
40
80
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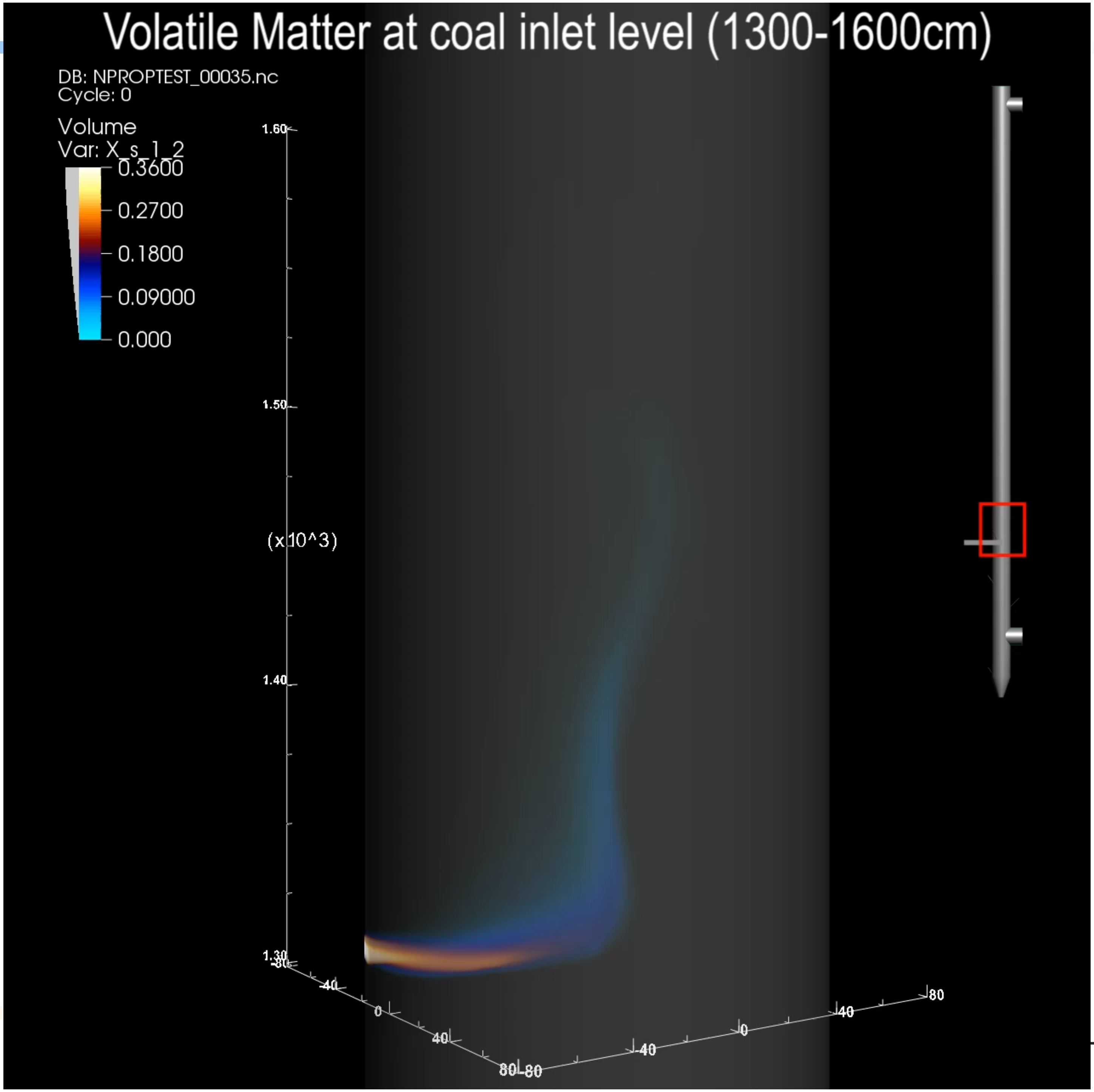
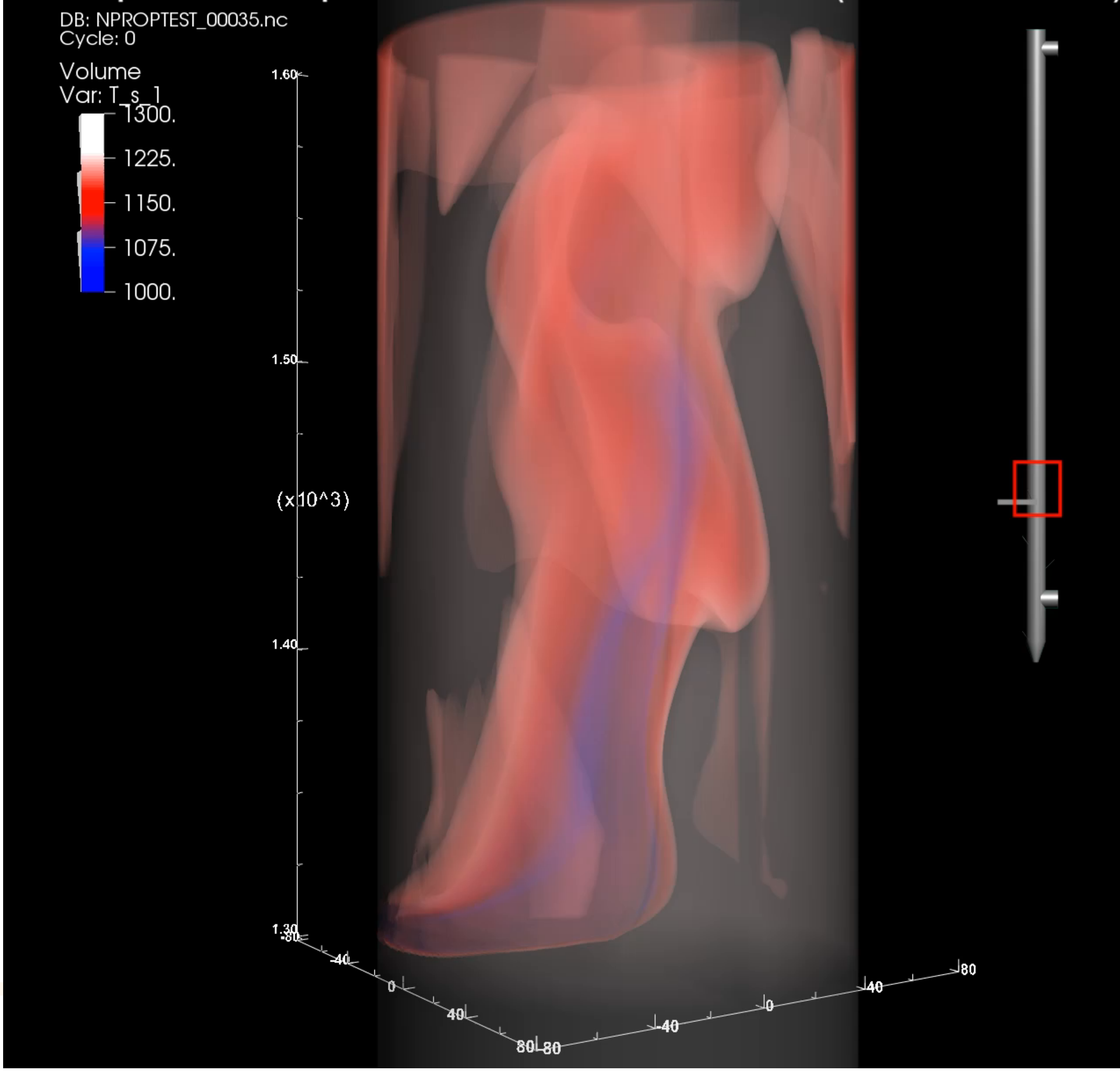
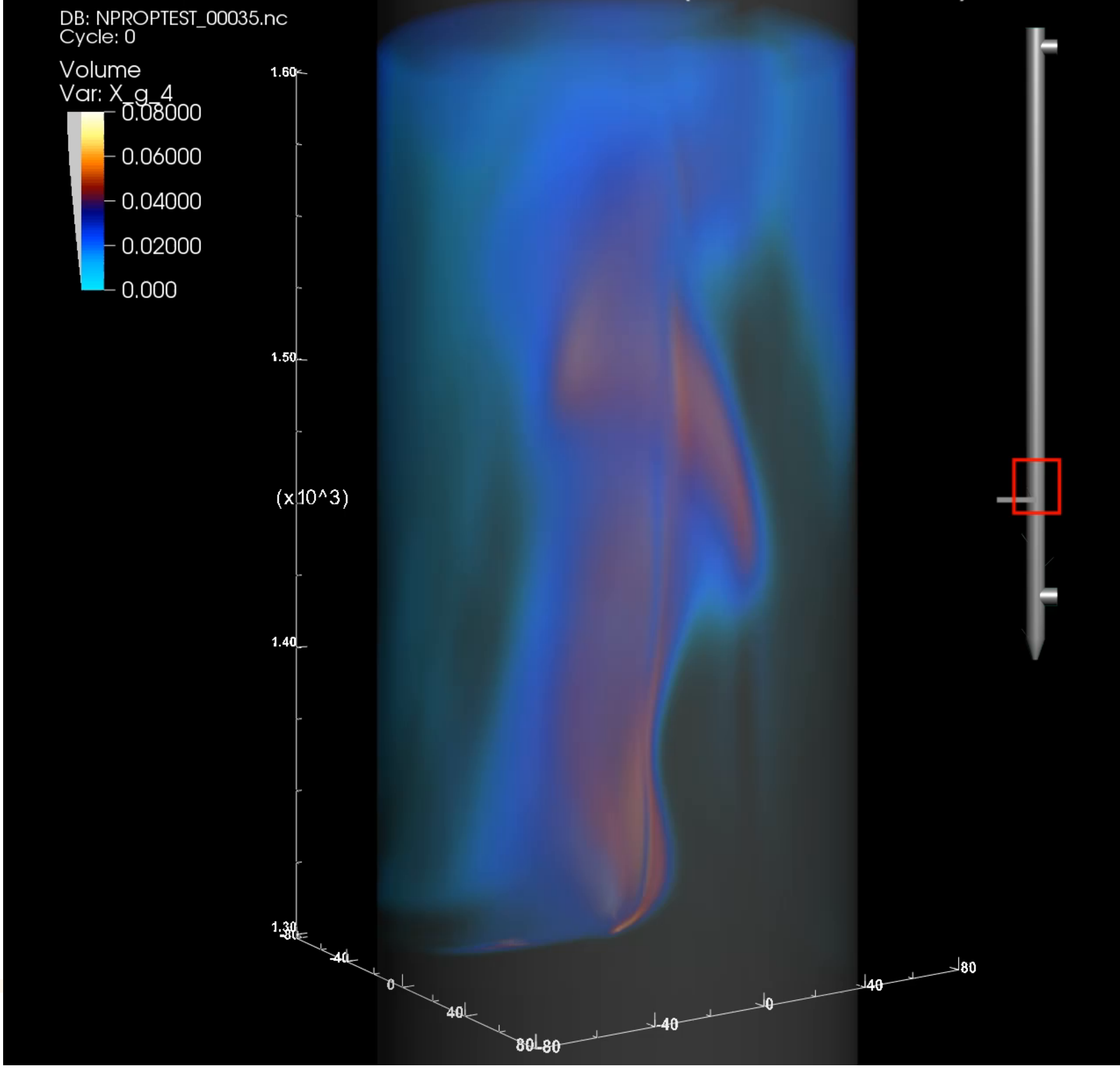


Volatile Matter at coal inlet level (1300-1600cm)
DB: NPROPTEST_00035.nc
Cycle: 0
Volume
Var: X_s_1_2
0.3600
0.2700
0.1800
0.09000
0.000
1.60
1.50
(x10^3)
1.40
1.30
-80
-40
0
40
80
-80
-40
0
40
80

Solid phase temperature at coal inlet level (1300-1600cm)

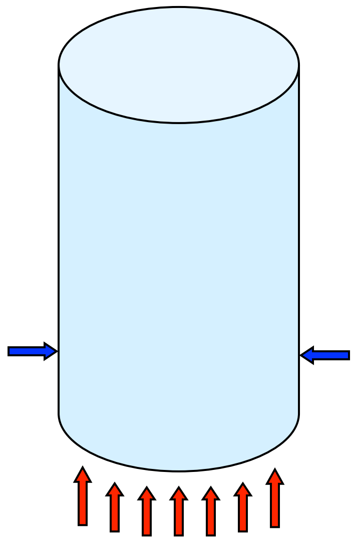


Methane at coal inlet level (1300-1600cm)



Case C: Reduced Configuration Simulation

- **Objective**
  - To better understand the coal jet penetration with high resolution simulation
  - To investigate the impact of grid resolution and numerical schemes
- **Simulation setup**
  - A section of a full-scale gasifier
  - Inflow from full-scale simulation

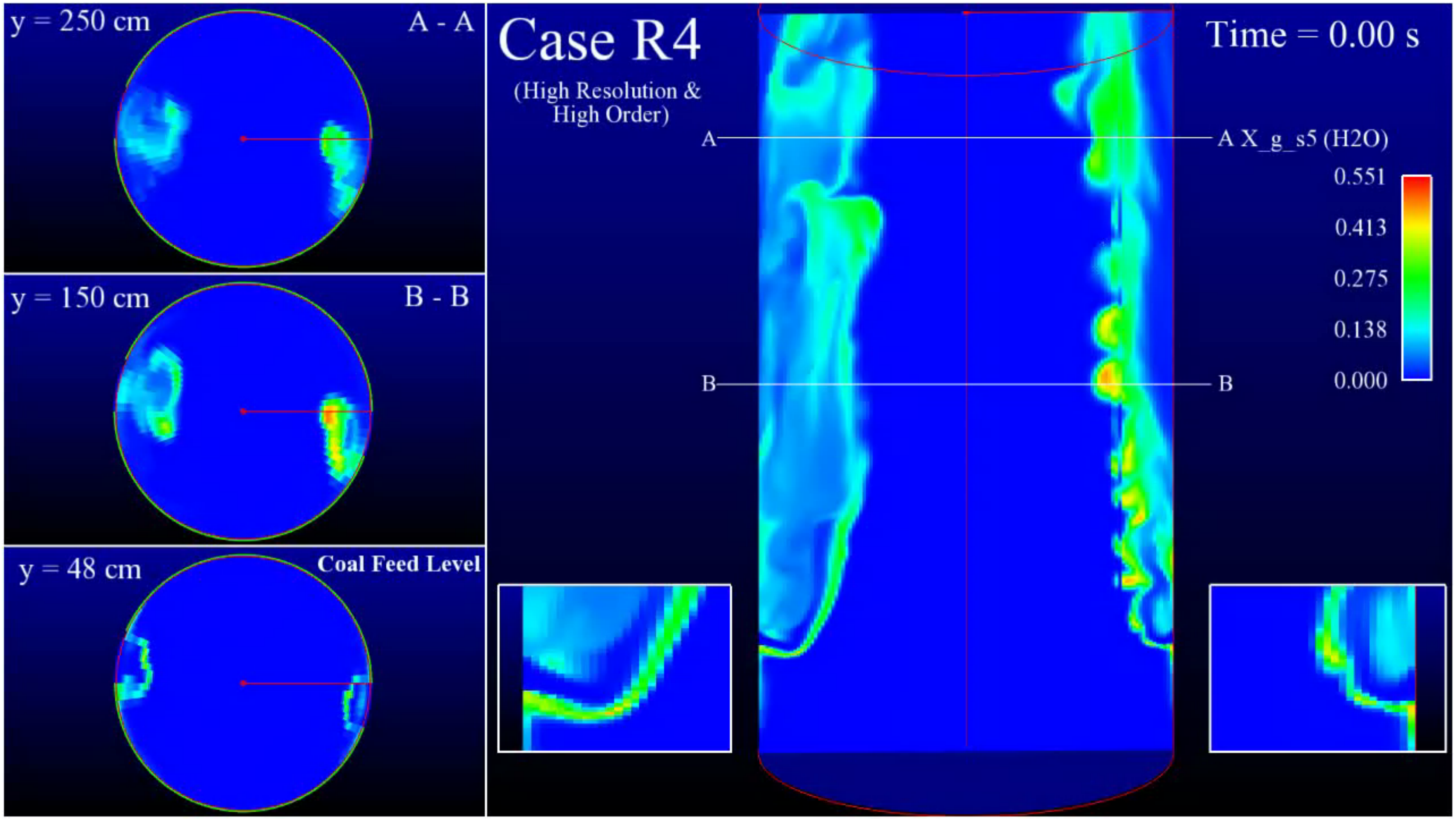


Case C: Simulated Cases

- **Summary of runs**
  - Three grid resolutions
  - Different numerical schemes
    - First order upwind vs. second-order superbee

Grid Resolution	Cell number (M)	Case Name	Discretization scheme
Coarse	0.35 (30x225x45)	CL	Low order
		CH	High order
Medium	0.7 (40x300x60)	ML	Low order
		MH	High order
Fine	2.4 (60x450x90)	FL	Low order
		FH	High order

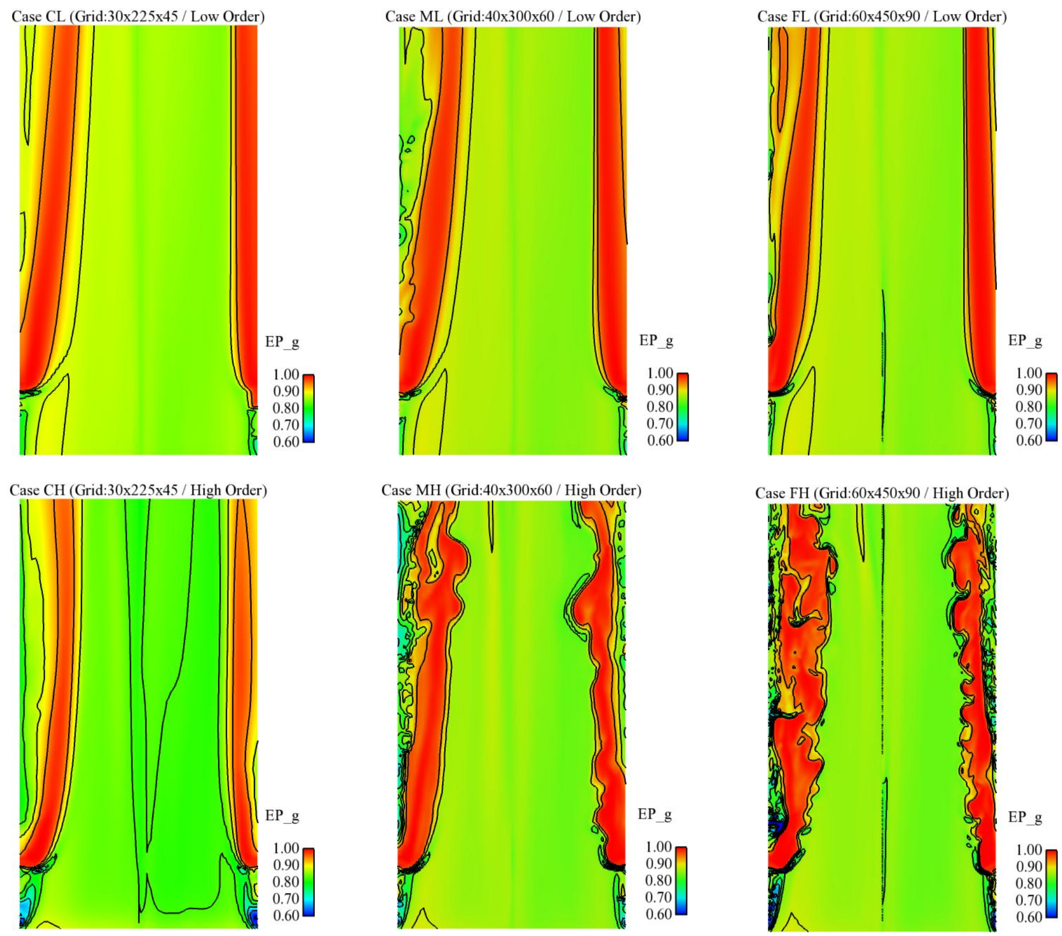
Case C: Transient Results



H2O mass fraction

H2O mass fraction

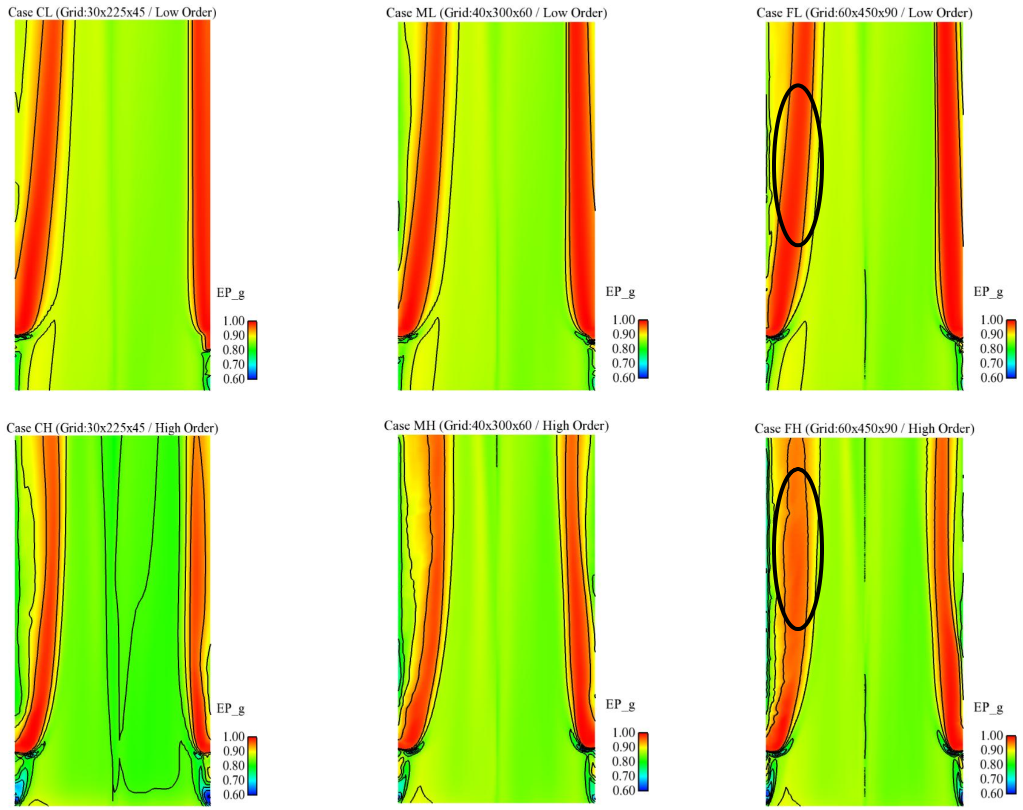
Case C: Transient Results



Voidage profiles for all cases along a clip plane aligned with two feed jets

H2O mass fraction

Case C: Time-averaged Results



Time-averaged voidage profiles for all cases along a clip plane aligned with two feed jets

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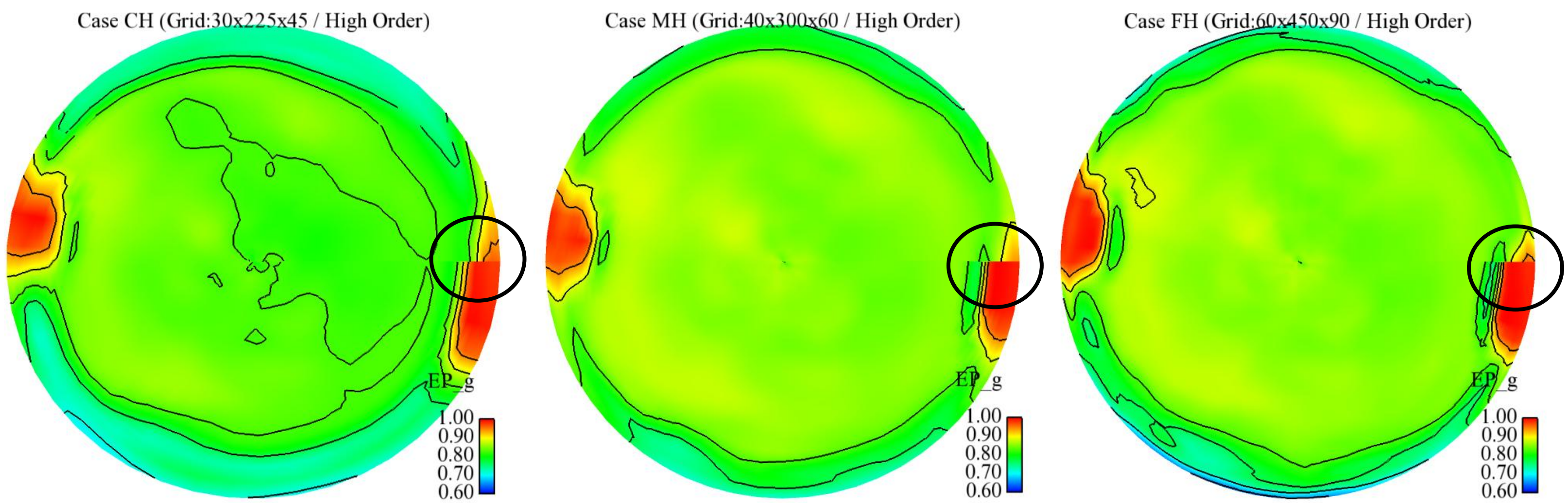
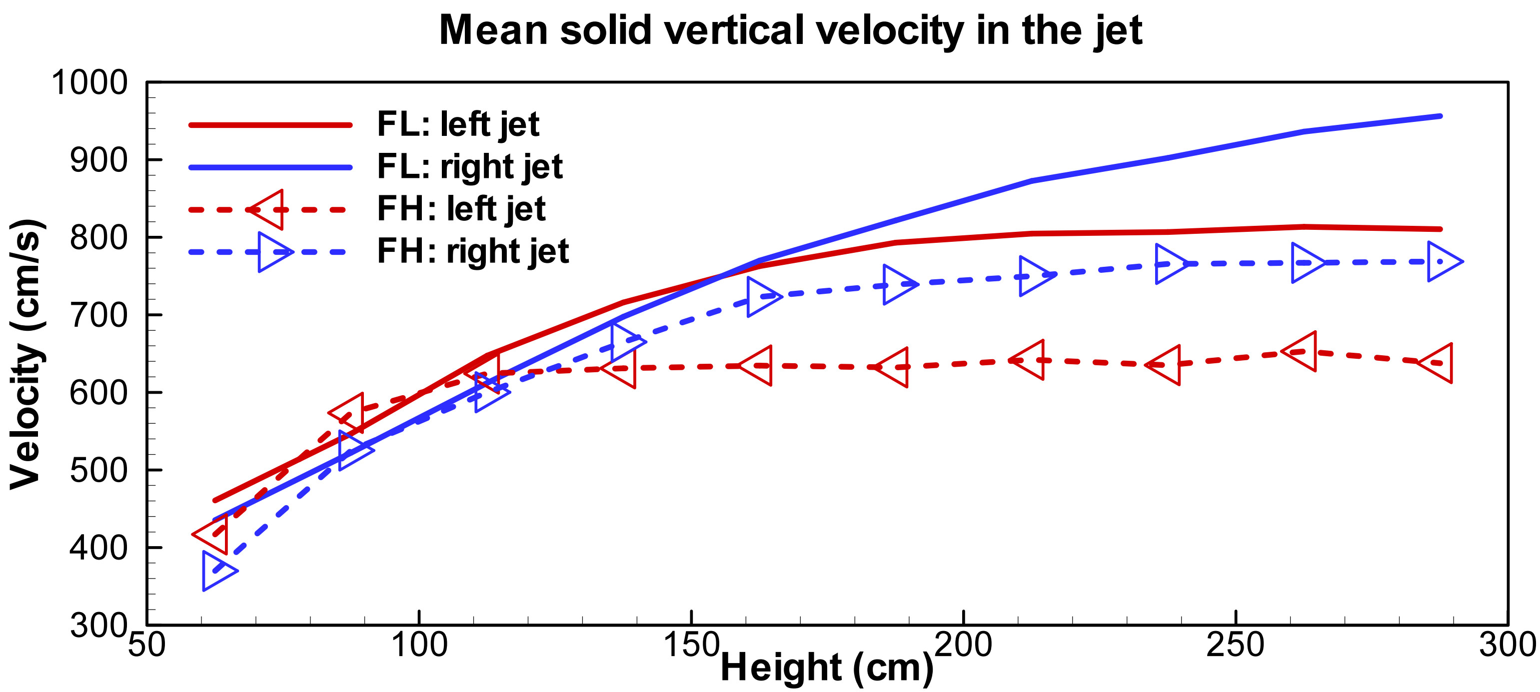
Case C: Time-averaged Results

- **Cross-sectional voidage**



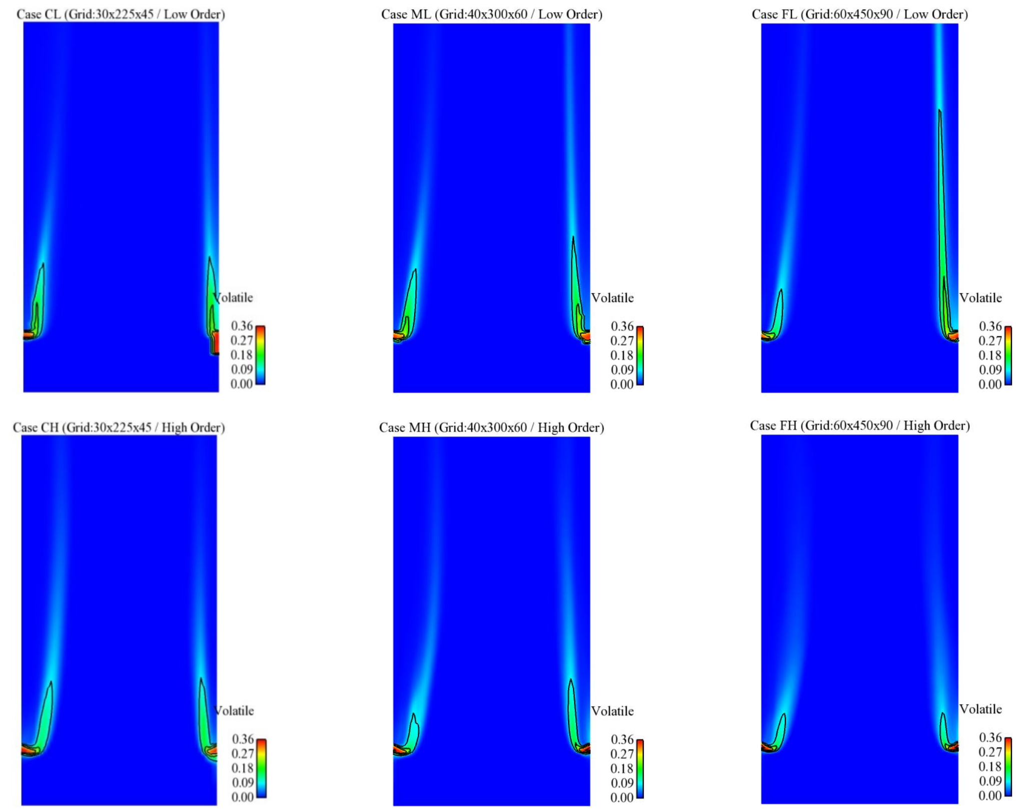
Time-averaged voidage profiles for cases with high-order scheme at the feed injection level

Case C: Coal Residence Time



Case #	CL	ML	FL	CH	MH	FH
Left jet (s)	0.363	0.367	0.361	0.360	0.407	0.418
Right jet (s)	0.381	0.355	0.354	0.430	0.392	0.394
Residence time (s)	0.371	0.363	0.359	0.391	0.401	0.408

Case C: Coal Devolatilization



Time-averaged mass fraction of volatile matter along a clip plane aligned with two feed jets

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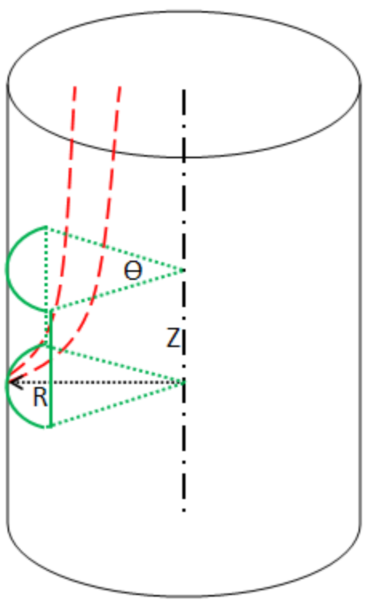
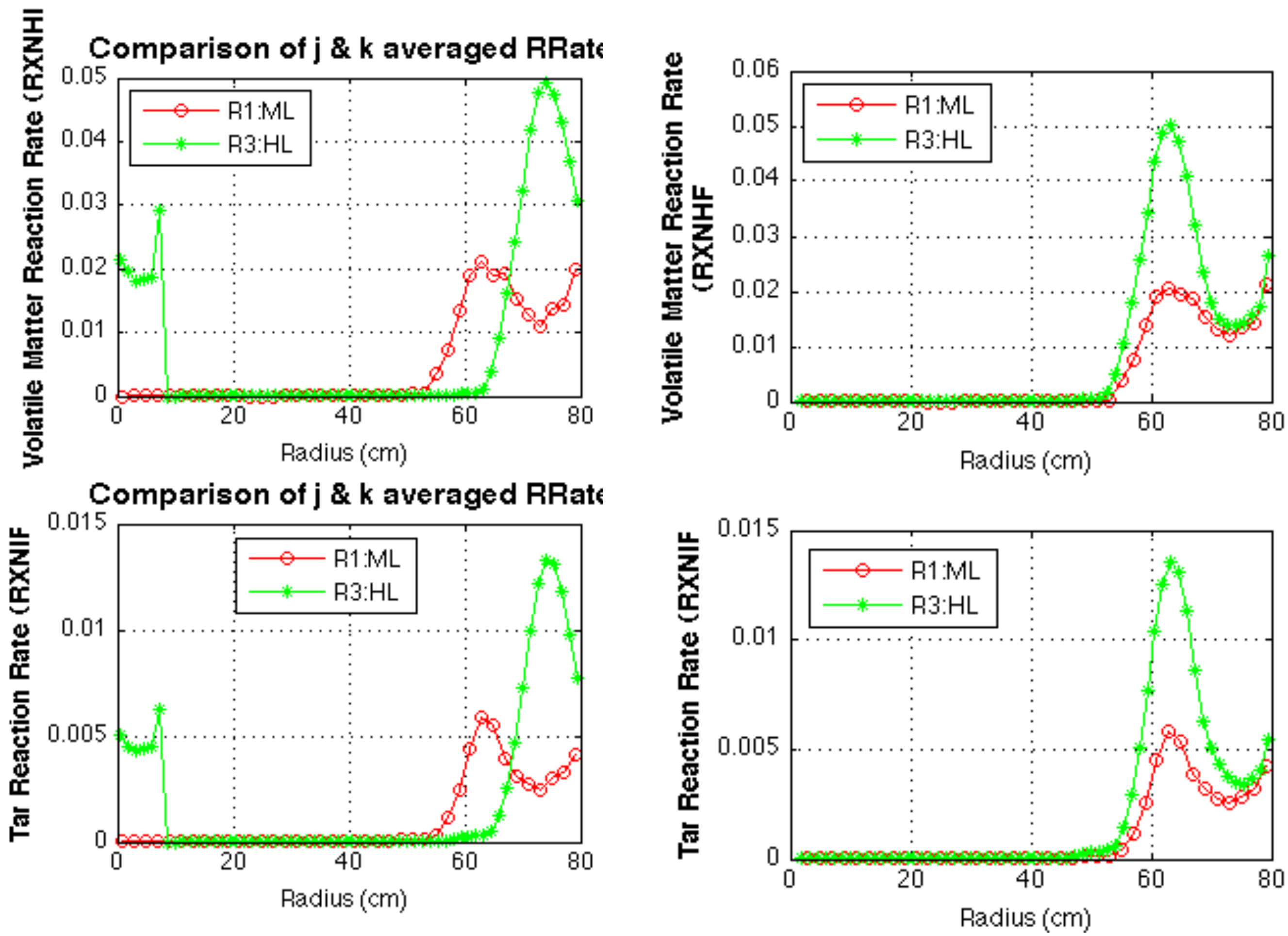
Case C: Influence Grid Resolution on Reaction Rates





Spatial-averaged radial profiles for instantaneous (left) and time-averaged (right) reaction rates

Conclusions

- **Demonstrated a first-of-its-kind high resolution gasifier simulation to address commercial scale industrial problem.**
- **High-order discretization scheme should be used to capture transient behavior.**
  - Might not be feasible for main stream applications
- **An adequately fine grid is needed to resolve the hydrodynamics & chemistry satisfactorily.**
- **The trade-off between accuracy and computational time must be taken into account for commercial scale simulations.**
- **Combine high and low resolution simulations for the design of commercial-scale gasifiers**

Future Work (2010)

- **Commercial Scale Configuration:**
  - Post-processing and data mining of Case A & B for quantitative analysis.
  - Provide design feedback to industrial collaborators.
  - Submit new INCITE proposal to request more time!
- **Reduced Configuration:**
  - Detailed analysis to quantify how grid resolution and numerical scheme affect reaction rates and species composition.
  - Subset case with further grid refinement (7.5 x particle size)
  - Compare across 4 distinct resolutions.

Publications

- Syamlal, M., C. Guenther, A. Gel, and S. Pannala (2010), In Proceedings of High Performance Computing: Clean Coal Gasifier Designs Using Hybrid Parallelization, Fluidization XIII 2010, Gyeong-ju, Korea, 2010.
- Li, T, A. Gel, M. Syamlal, C. Guenther, and S. Pannala, “High Resolution Simulations Of Coal Jets In A Gasifier” 21st International Symposium on Chemical Reaction Engineering (submitted for peer review evaluation).
- Gel, A., C. Guenther, R. Sankaran, S. Pannala, M. Syamlal, and T. J. O’Brien (2009), “Accelerating Clean Coal Gasifier Designs with High Performance Computing”, In the Proceedings of the 21st International Conference on Parallel CFD, 18–22 May 2009, Moffett Field, California, USA.
- Syamlal, M., C. Guenther, A. Gel, and S. Pannala (2009), “Advanced coal gasifier designs using large-scale simulations “, Journal of Physics: Conference Series, Volume 180, 012034 (10pp) doi: 10.1088/1742-6596/180/1/012034 180.

Acknowledgments

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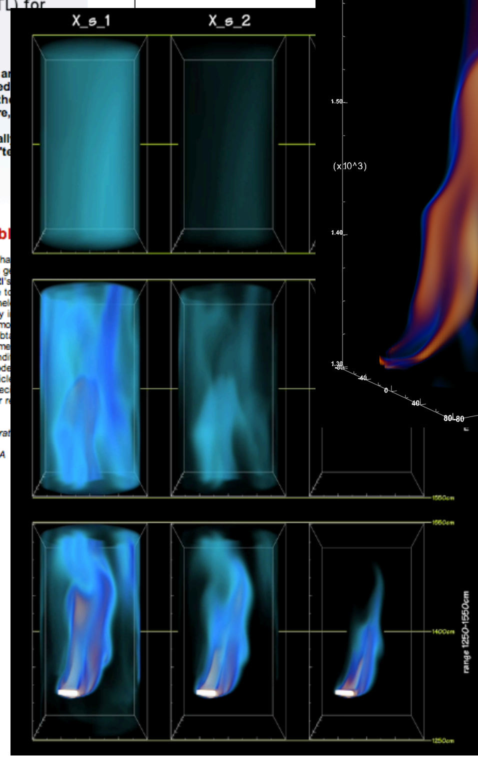
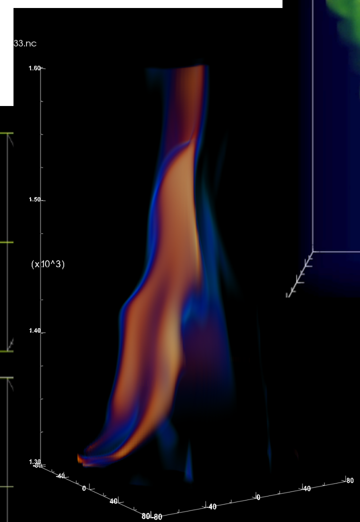
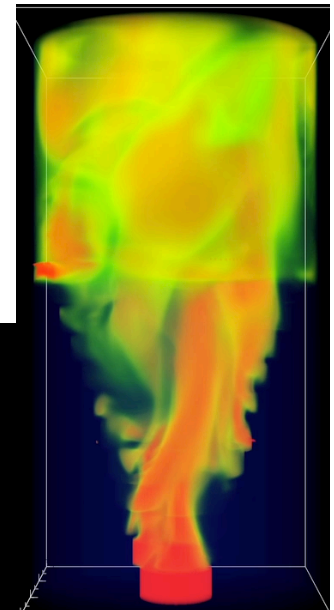
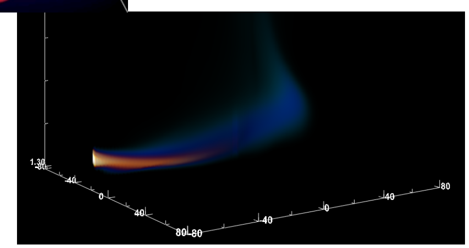
Questions?









Visit MFIX website for more information

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