UT-BATTELLE

Understanding the Interactions between Hydrodynamics and Chemistry in Coal Gasifier Simulations

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Acknowledgments: MFIX Team

NETL

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Outline of today's talk

- **Motivation**
- **Model background**
- **Problem setup**
  - **Ozone Case**
  - **Simple Coal Chemistry**
  - **Full Coal Chemistry**
- **Coupling of hydrodynamics, heat-release and chemistry**
- **Conclusions and future work**

Motivation

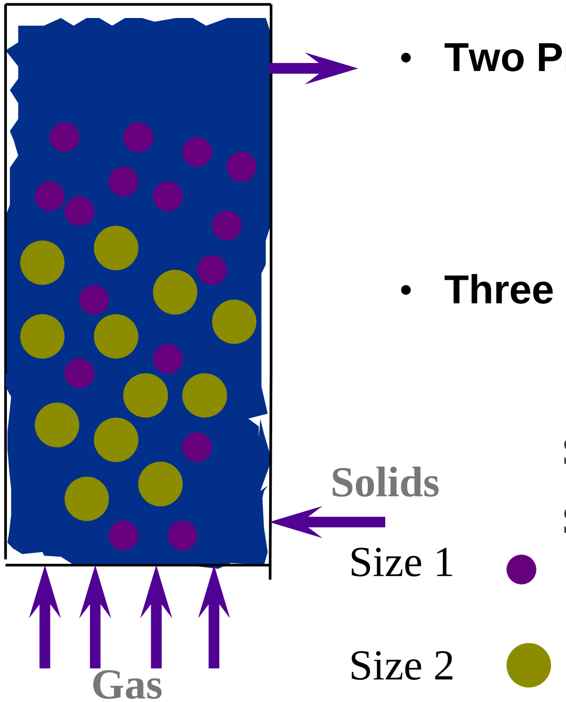
- **Develop a systematic procedure to understand the interaction between different non-linear processes (convection, reactions, diffusion, phase change, heat & mass transfer)**
  - **Cause and effect?**
  - **Is it even possible to unravel the behavior of such complex systems?**
- **Critical for design**
  - **The desirable conversion is dependent on the time-scales of the various processes but also the spatiotemporal evolution of the field variables**
    - **Exothermic reactions, solids distribution, thermal expansion etc.**
  - **The effect of inlets and boundary conditions**
  - **What is the optimal size of the reactor?**
    - **Reactor height, location/area/mass-flow of the inlets etc.**
  - **Insights into scaling?**
- **Enormous amount of data from large simulations**
  - **Knowledge discovery**
  - **Aid development of reduced-order models**
  - **Aid experiments**
  - **Current evaluation of accuracy might be limiting**

MFIX Simulation Package

- **General multiphase fow CFD code which couples hydrodynamics, heat & mass transfer and chemical reactions**
- **SMP, DMP and Hybrid Parallel code which runs on many platforms including Beowulf clusters**
- **Open-source code and collaborative environment (http://www.mfix.org or http://mfix.netl.doe.gov)**
- **Over 1500 researchers from over 500 institutions around the world**

2007

Multiphase Formulation



- **Two Phases**

Fluid

Solids

- **Three phases**

Fluid

Solids - 1

Solids - 2

• **Details of flow field and particle interaction have been averaged out.**
• **Account for the information lost due to averaging through the use of *constitutive equations***

Continuity Equation

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

Momentum Equation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \bar{\bar{S}}_m + \sum_{l=1}^{M} \vec{I}_{ml} + \vec{f}_m$$

Stresses

Interaction Term

Granular Stresses are modeled by the kinetic theory of granular material in the viscous regime and plasticity theory in the plastic regime

Drag law describes the interaction between the gas and the particles

Carbonaceous Chemistry for Continuum Modeling (C3M)

Excellence in Technology Transfer Award 2008

- **Devolatilization**

  HF: Volatile Matter $\rightarrow \alpha_d$ Tar + $\beta_d^{CO}CO + \beta_d^{CO2}CO_2 + \beta_d^{CH4}CH_4 + \beta_d^{H2}H_2 + \beta_d^{H2O}H_2O$

- **Cracking** *IF:* Tar $\rightarrow \alpha_c C + \beta_c^{CO}CO + \beta_c^{CO2}CO_2 + \beta_c^{CH4}CH_4 + \beta_c^{H2}H_2 + \beta_c^{H2O}H_2O$

- **Drying** *GF:* Moisture (coal) $\rightarrow H_2O$

- **Water-gas shift reaction** *EF:* $CO + H_2O \leftrightarrow CO_2 + H_2$

- **Gasification**

  BF: $C + H_2O \leftrightarrow CO + H_2$

  CF: $C + CO_2 \leftrightarrow 2CO$

  DF: $\frac{1}{2}C + H_2 \leftrightarrow \frac{1}{2}CH_4$

Combustion

0F: $H_2 + 2O_2 \rightarrow H_2O$

1F: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

2F: $CO + \frac{1}{2}O_2 \rightarrow CO_2$

AF: $2C + O_2 \rightarrow 2CO$

Carbonaceous Chemistry for Continuum Modeling (C3M)

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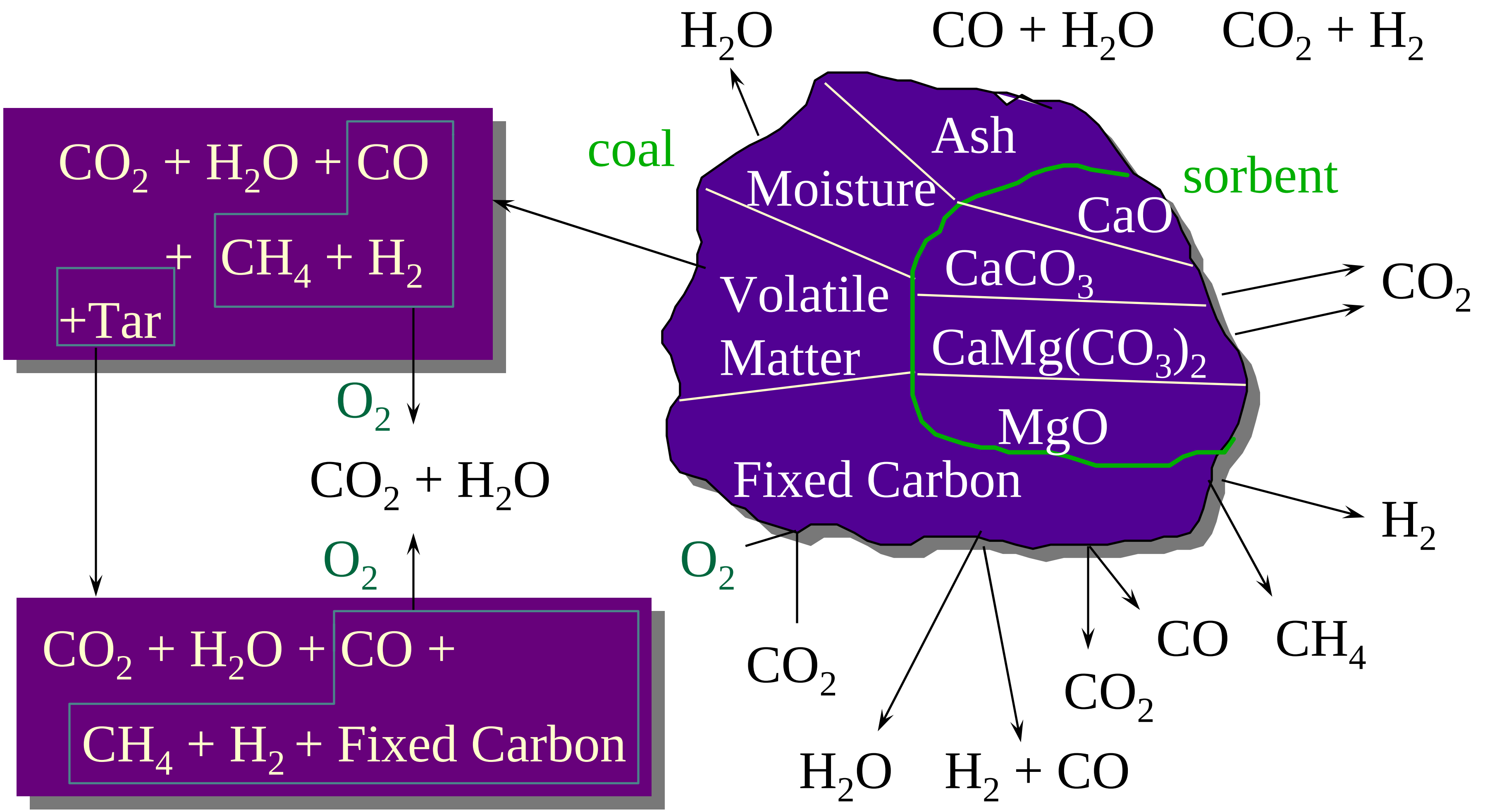

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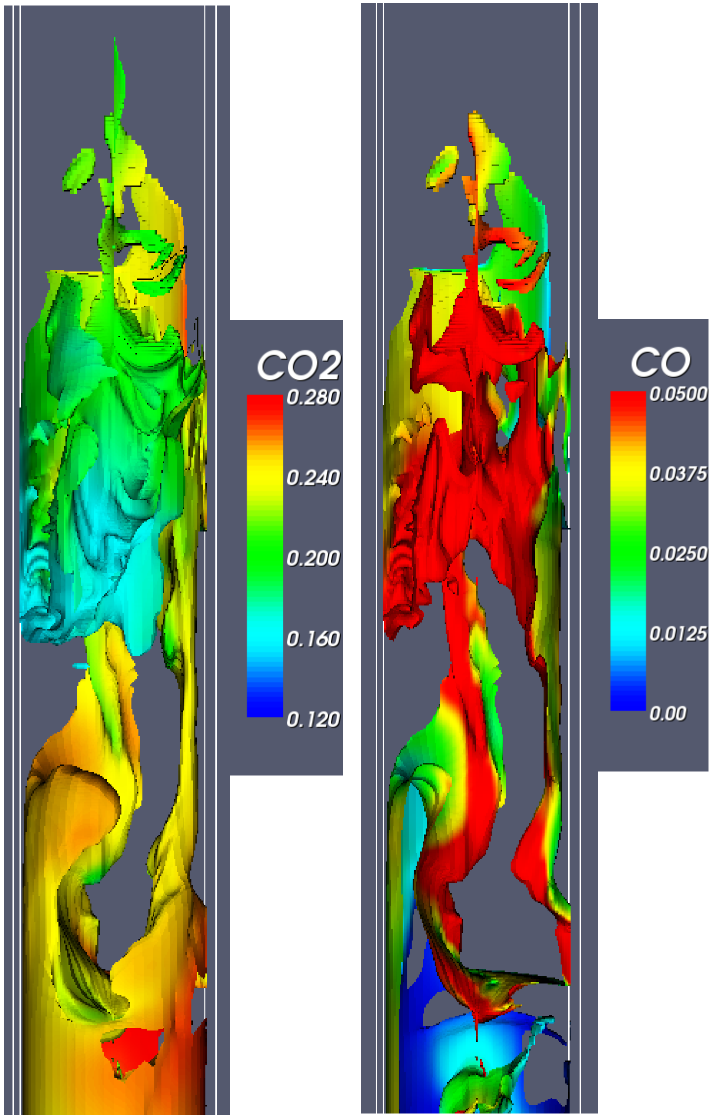
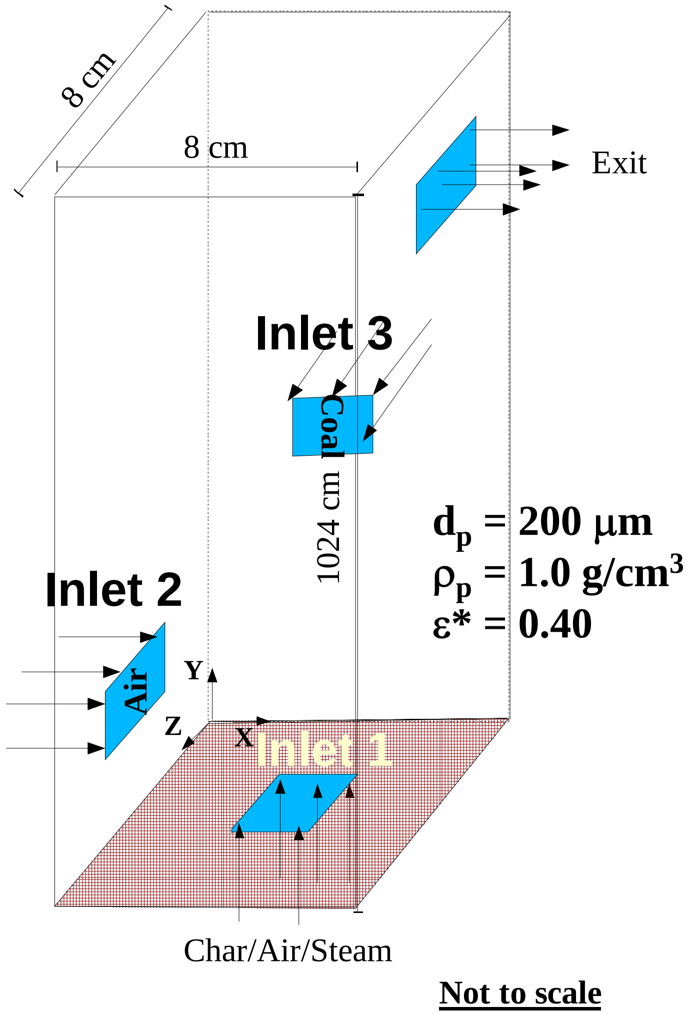
Coal Gasification Simulations

- **We are conducting high resolution gasifier simulations**
  - **2 week run using 2048 processors for a 10M grid**
- **Earlier simulations led to design modifications**
  - **Lower riser gas and solids velocities**
  - **Down flow at the wall (clusters are present)**
  - **Improved mixing in the riser**
- **Coal gasifiers are integral part of current clean coal technologies**

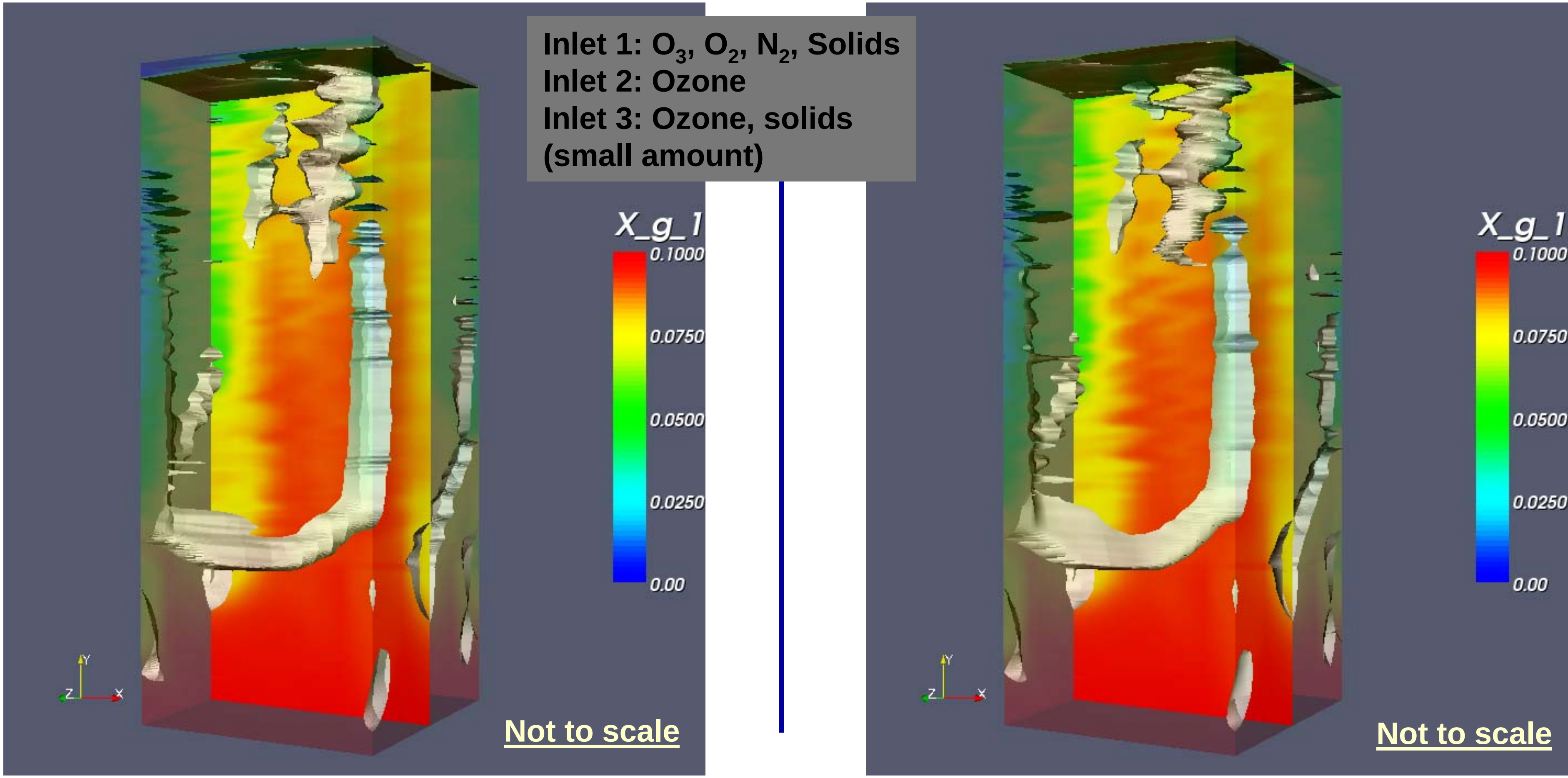


Simulation Configuration



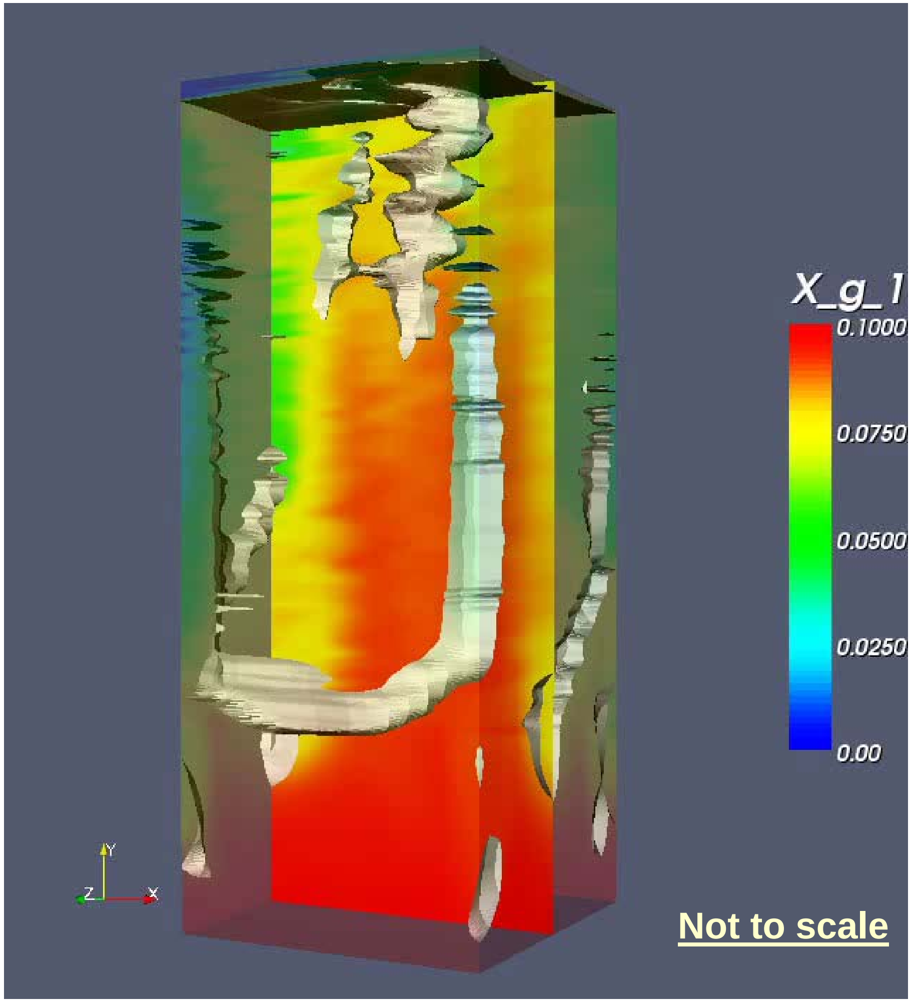
- Char/Air/Steam inlet and Exit - 4x4 cm
- Coal and Air inlets – 2x2 cm
- Cartesian mesh
- Cases Studied:
  - Case A: Ozone decomposition
  - Case B: Char combustion
  - Case C: Complex gasification chemistry
- Different resolutions
  - 0.25M cells: Cases A, B, and C
    - 2-3 weeks run-time for 15s on 16-32 processors (AMD Cluster)
  - ~2M cells: Case C
    - 10-days run-time for 15s on 256-512 processors (CRAY XT4)
  - ~10M cells: Case C
    - 1-week run-time for 5s on 1024-2048 processors (CRAY XT4)

Ozone concentration along with solids contours (Case A – Ozone Decomposition)

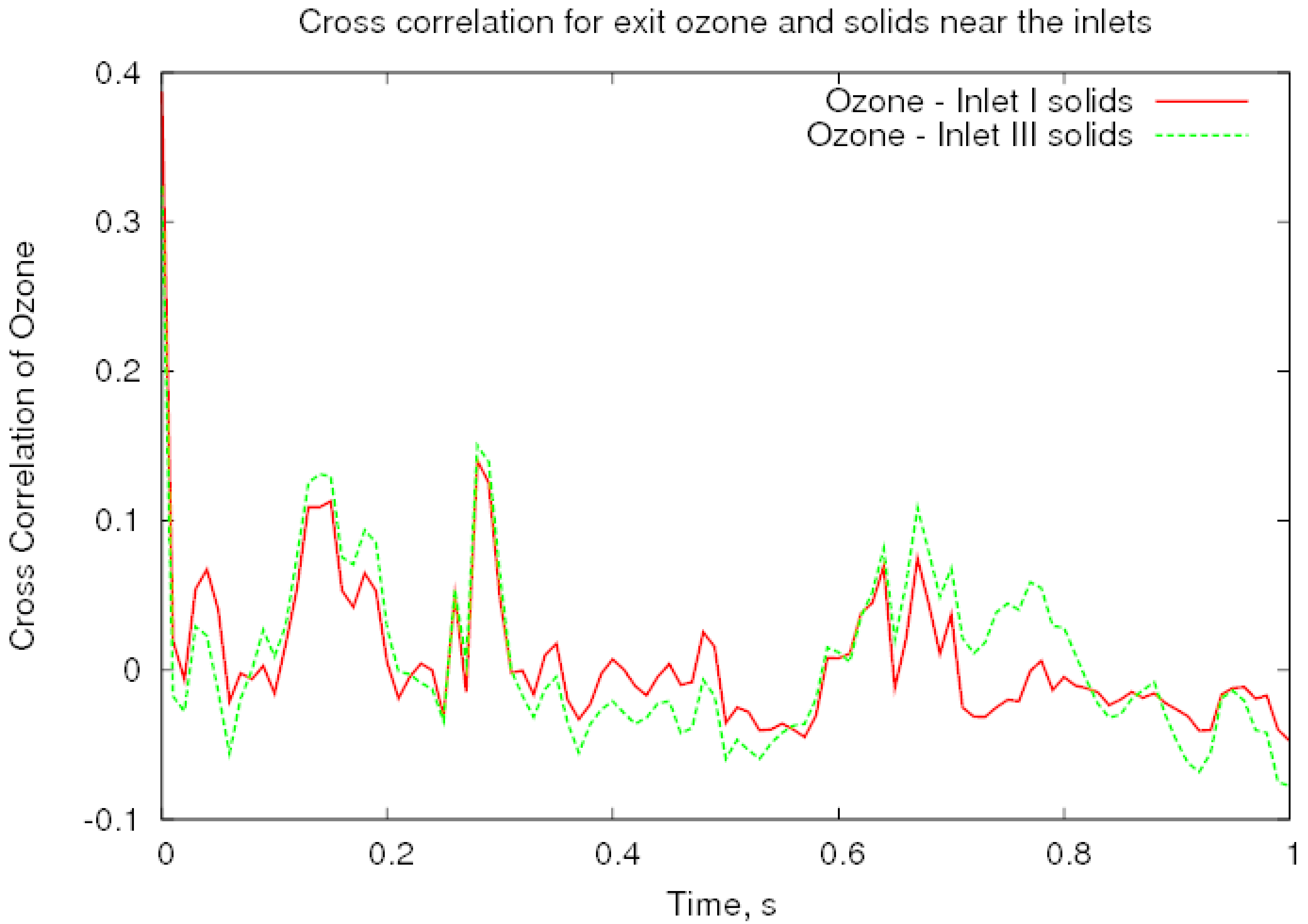


- **Solids accumulate primarily at corners and top**
- **Ozone conversion is strongly correlated to solids presence**

Ozone concentration along with solids contours (movie)



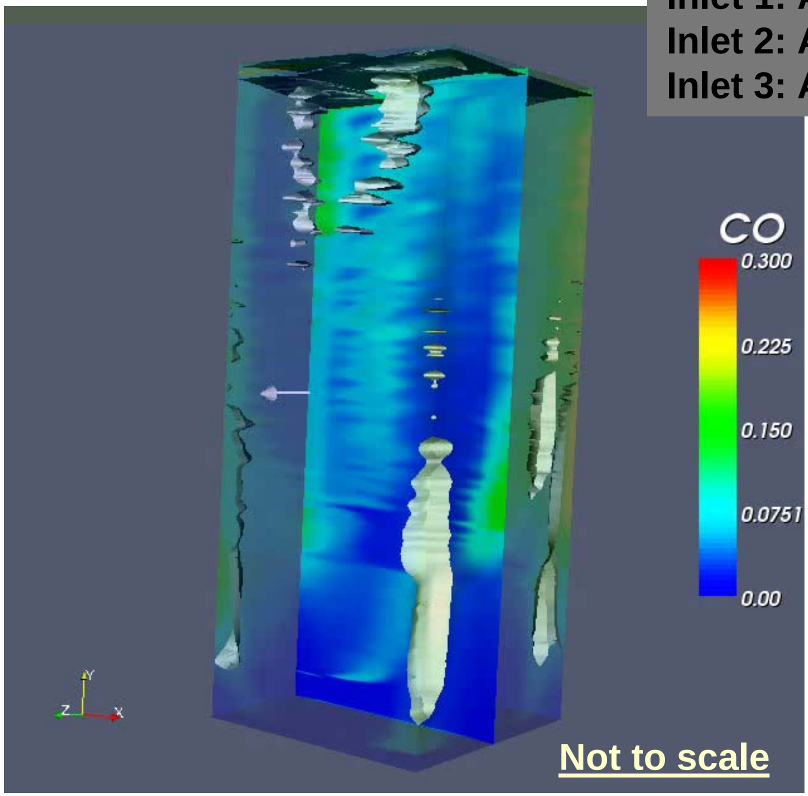
Cross-correlation

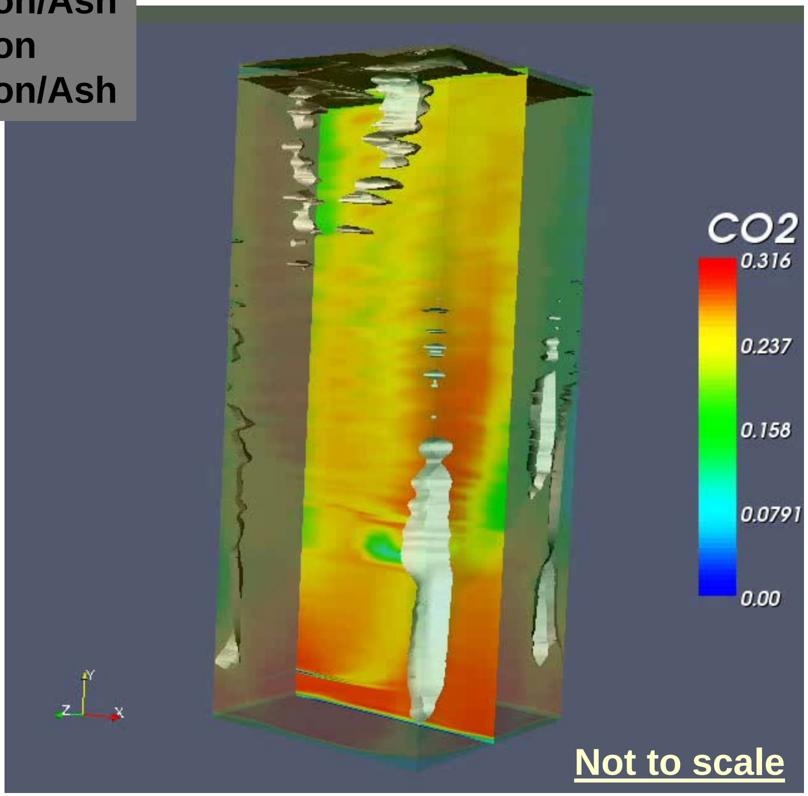


- **Weak correlation between the exit ozone and inlet solids**
- **Too many complex interactions in the reactor**

CO and CO_2 along with solids contours (Case B – Char Combustion)

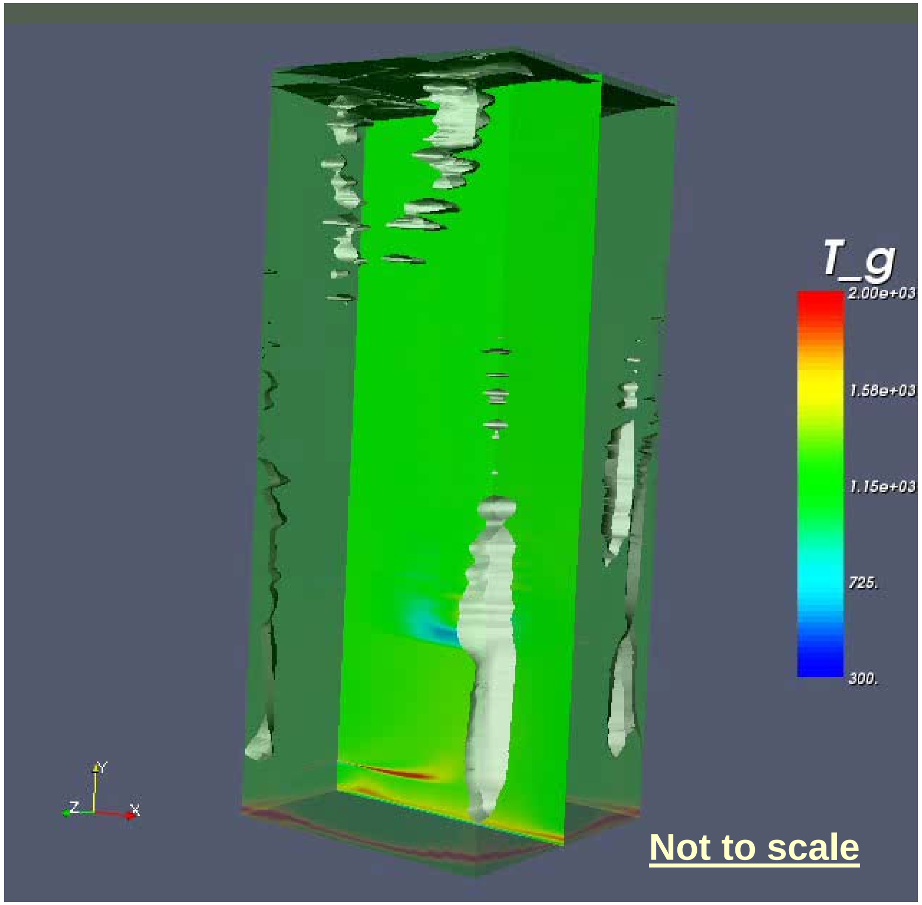
Inlet 1: Air, Carbon/Ash
Inlet 2: Air, Carbon
Inlet 3: Air, Carbon/Ash





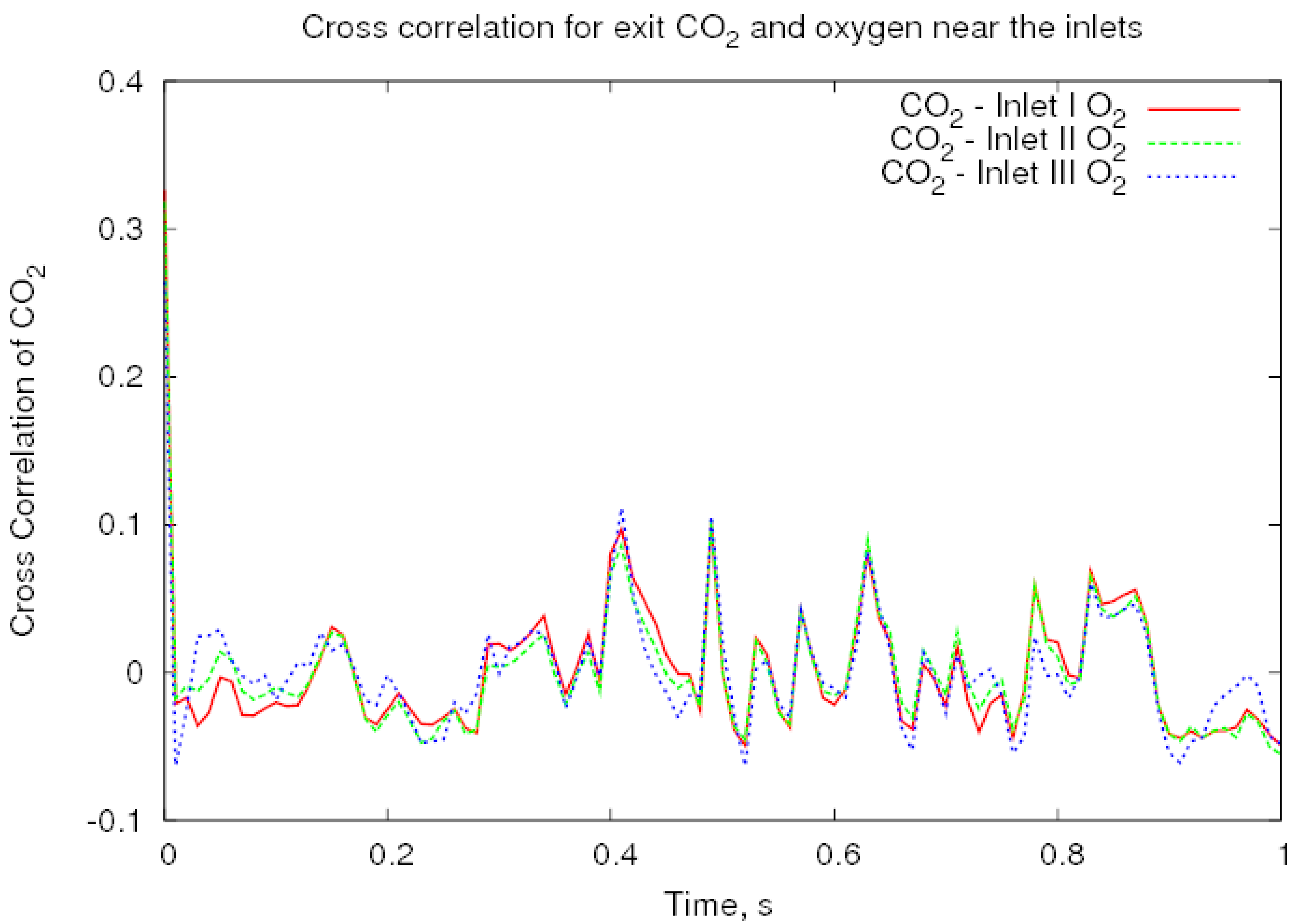
- **Solids accumulate primarily at corners in the lower domain and top wall**
- **Higher CO and lower CO_2 in the vicinity of solids**

Gas Temperature along with solids contours (Case B – Char Combustion)



- **Solids accumulate primarily at corners in the lower domain and top wall**
- **Weak correlation between the solids and gas-temperature**

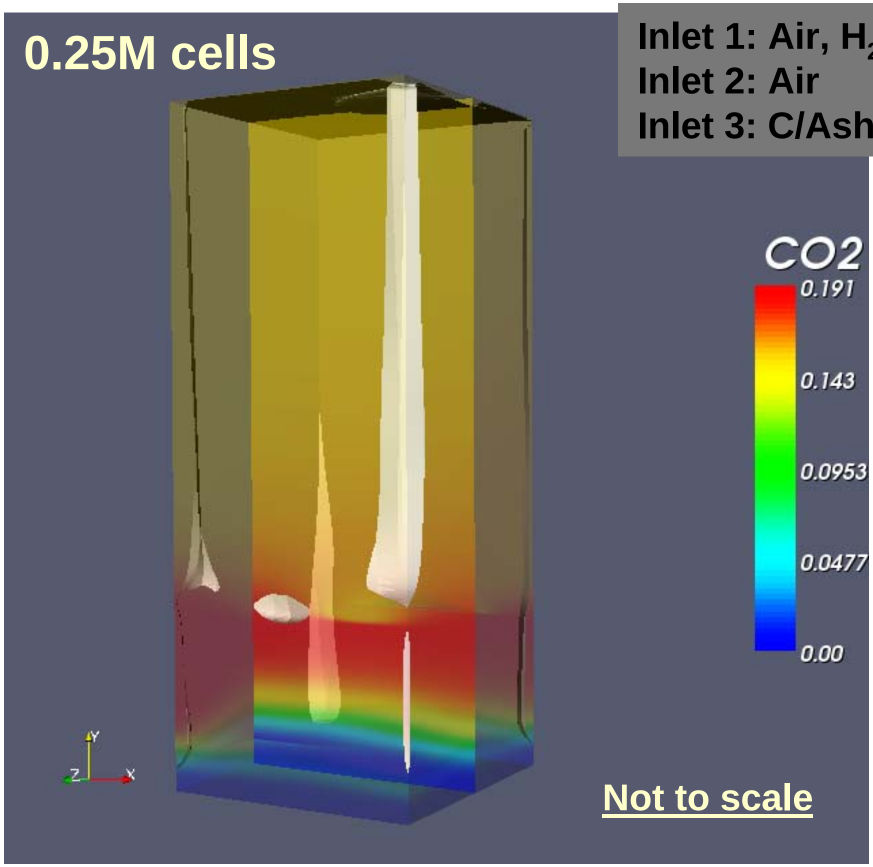
Cross-correlation

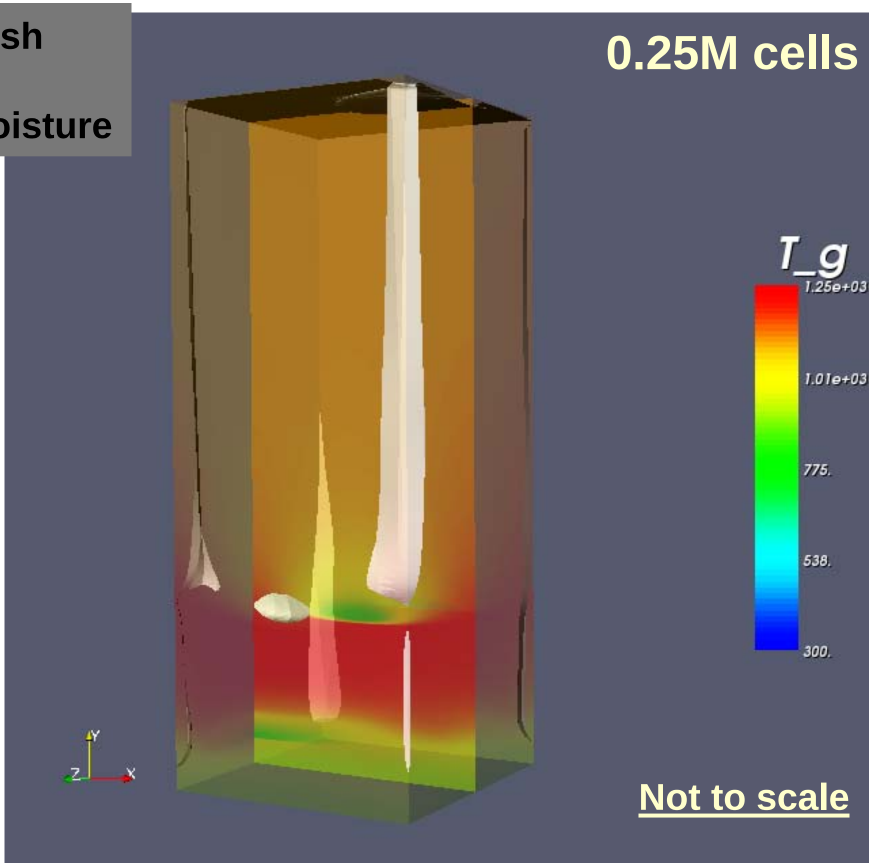


- **Weak correlation between the exit CO_2 and inlet O_2**
- **Too many complex interactions in the reactor**
- **Correlation seems to be weaker than O_3**

Gas Temperature and CO_2 along with solids contours (Case C - C3M Module)

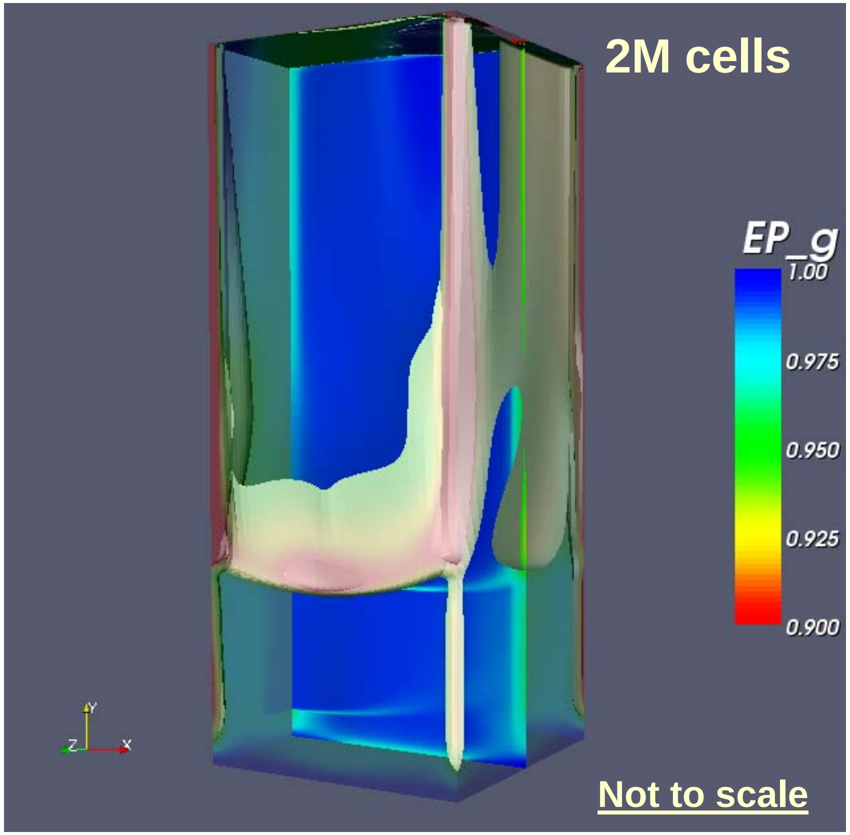
Inlet 1: Air, H_2O, C/Ash
Inlet 2: Air
Inlet 3: C/Ash/VM/Moisture

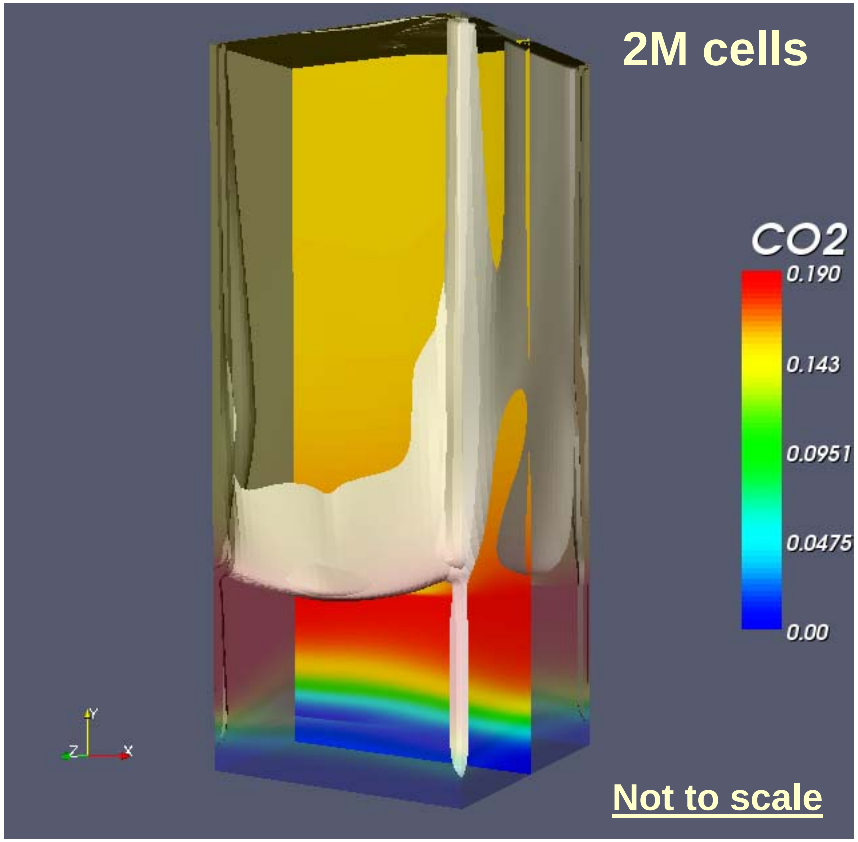




- **Solids accumulate primarily at the corners and top wall**
- **Gas temperature and CO_2 are strongly correlated**

Void Fraction and CO_2 along with solids contours (Case C - C3M Module)





- **Resolution provides better details**
- **Qualitative trends remain the same except for higher solids loading at the walls**

Conclusions

- **Geometry effects (e.g. square cross-section) seem to dominate**
  - **Significant solids presence near the corners**
- **The interaction between the various processes seems to be quite complicated**
  - **2-point correlations might not be sufficient to understand the complete picture unless they are very local and targeted**
  - **Possibly look at m-point correlations, transfer entropy and other tools from information theory**
  - **Integrated residence times w.r.to various variables**
  - **Direct probing of the data through reconstruction of the steepest gradient surfaces and understanding the role of the different terms might be needed**
- **Any of these analysis tools have to be related to scaling and sizing to be of use to reactor design**

Ongoing and Future work

- **Continue development of the analysis tools and protocols while improving the turn-around time for the simulations**
- **Migrate the analysis to commercial scale gasifier**
- **Important design questions that need to be answered:**
  - **Effect of coal jet penetration on SynGas composition**
  - **Reactor length/diameter**
  - **Coal feed rate**
  - **Solids recirculation rate**
  - **Effect of recycled syngas**

Thank you for your attention!!

http://www.mfix.org

http://mfix.netl.doe.gov