Understanding the Interactions between Hydrodynamics and Chemistry in Coal Gasifier Simulations

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Sponsors: DOE Fossil Energy
Computing Resources: Clusters and NCCS CRAY XT4
Acknowledgments: MFIX Team
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 flow 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
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
\[
\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \vec{S}_m + \sum_{l=1}^{M} \vec{I}_{ml} + \vec{f}_m
\]

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)

- **Devolatilization**
  
  \[ HF: \text{Volatile Matter} \rightarrow \alpha_d \text{Tar} + \beta_d \text{CO} + \beta_d \text{CO}_2 + \beta_d \text{CH}_4 + \beta_d \text{H}_2 + \beta_d \text{H}_2\text{O} \]

- **Cracking**
  
  \[ IF: \text{Tar} \rightarrow \alpha_c \text{C} + \beta_c \text{CO} + \beta_c \text{CO}_2 + \beta_c \text{CH}_4 + \beta_c \text{H}_2 + \beta_c \text{H}_2\text{O} \]

- **Drying**
  
  \[ GF: \text{Moisture (coal)} \rightarrow \text{H}_2\text{O} \]

- **Water-gas shift reaction**
  
  \[ EF: \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \]

- **Gasification**
  
  \[ BF: \text{C} + \text{H}_2\text{O} \leftrightarrow \text{CO} + \text{H}_2 \]

  \[ CF: \text{C} + \text{CO}_2 \leftrightarrow 2\text{CO} \]

  \[ DF: \frac{1}{2}\text{C} + \text{H}_2 \leftrightarrow \frac{1}{2}\text{CH}_4 \]

- **Combustion**
  
  \[ 0F: \text{H}_2 + 2\text{O}_2 \rightarrow \text{H}_2\text{O} \]

  \[ 1F: \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \]

  \[ 2F: \text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \]

  \[ AF: 2\text{C} + \text{O}_2 \rightarrow 2\text{CO} \]
Carbonaceous Chemistry for Continuum Modeling (C3M)
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

Cross correlation for exit ozone and solids near the inlets

- 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)

- Solids accumulate primarily at corners in the lower domain and top wall
- Higher CO and lower CO$_2$ in the vicinity of solids

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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)

- Solids accumulate primarily at the corners and top wall
- Gas temperature and CO$_2$ are strongly correlated
Void Fraction and CO₂ 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.t. 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