7th International Freiberg/Inner Mongolia Conference
Coal Conversion and Syngas
7-11 June 2015
Huhhot, Inner Mongolia, China
Numerical Simulation of a New Reactor for the In-Situ Measurement of Char Particle Conversion

June 9, 2015

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Motivation

- In entrained-flow gasification, char conversion occurs at high temperatures, high pressures.
- Fundamental knowledge processes at single particles necessary for advanced sub model development.
- Drop tube and TGA experiments are not able to reflect process conditions (isolated particles, defined gas flow, high temperature/pressure).
- CFD modeling of isolated reacting particles helps to understand basic physics, but need intensive validation.
HITECOM (High Temperature Conversion Optical Measurement)

- Alternative approach: in-situ measurements of isolated particles at defined pressures, temperatures, and gas flow velocity
- Joint project with Friedrich Schiller University Jena
- Reactor allows for high temperature (up to 1400 K) and high pressure (up to 40 bar)
- In-situ optical measurement of temperature and concentration around isolated, reacting particles allows for fundamental analysis of char conversion and provides validation data for particle-resolved CFD modeling
Content

• HITECOM Reactor
• Numerical model
• Results for numerical simulation
• Conclusion/Outlook
HITECOM Reactor

Geometry for Revision 1

Geometry for Revision 4
Numerical Model

- ANSYS-Fluent 15.0
- Steady-state
- Non-reacting flow with heat transfer
- Standard k-ε turbulence model, standard wall
- Different radiation models tested
- Second order upwind
Computational Grid

- Structure mesh with approx. 3 Mil. cells
- O-grid for pipes
First Results without Radiation and Gravity

- Gas properties under operation conditions (constant density)
- Wall Temperature unknown, defined a cooling coat with $T_{\text{ext}} = 300\text{K}$

\[
\dot{q} = \frac{1}{\frac{1}{h} + \frac{L}{\lambda}} (T_{\text{ext}} - T_{\text{w}})
\]

Simulation plan

<table>
<thead>
<tr>
<th>Modification</th>
<th>Pressure</th>
<th>Particle / Pipe Reynolds Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rev. 1</td>
<td>1.01 bar (1 atm)</td>
<td>10 / 155</td>
</tr>
<tr>
<td>Rev. 4</td>
<td>40 bar</td>
<td>100 / 1550</td>
</tr>
</tbody>
</table>
Wall Temperature

Geometry and wall temperature of Rev. 1

Geometry and wall temperature of Rev. 4
Velocity Magnitude in Symmetric Plane Rev. 1
Temperature Distribution in Symmetric Plane Rev. 1

- **Graph 1:**
  - **Conditions:** $p = 1$ atm, $Re = 10 / 155$, $c = 0.71$ m/s
  - **Temperature Range:** 1000 to 1400 K

- **Graph 2:**
  - **Conditions:** $p = 1$ atm, $Re = 100 / 1550$, $c = 7.1$ m/s
  - **Temperature Range:** 1000 to 1400 K

- **Graph 3:**
  - **Conditions:** $p = 40$ bar, $Re = 10 / 155$, $c = 0.018$ m/s
  - **Temperature Range:** 1000 to 1400 K
Velocity Magnitude and Temperature Distribution in Symmetric Plane Rev. 4
Reference Velocity and Temperature Plot in Radial Position

- Normalized Velocity vs. Radial Position, m
  - Three curves for different pressures and Reynolds numbers:
    - Red: p = 1 atm, Re = 10
    - Green: p = 1 atm, Re = 100
    - Blue: p = 40 bar, Re = 10
    - Orange: p = 40 bar, Re = 100

- Temperature vs. Radial Position, m
  - Three curves for different pressures and Reynolds numbers:
    - Red: p = 1 atm, Re = 10
    - Green: p = 1 atm, Re = 100
    - Blue: p = 40 bar, Re = 10
    - Orange: p = 40 bar, Re = 100
Heat Transfer Tests

- P-1 and DO radiation models take gas-phase and surface radiation into account
- The P-1 model tends to over-predict radiative fluxes from localized heat sources or sinks (Fluent Theory Guide), but is less computational expensive
- Test for non-uniform temperature distribution of walls

Simulation plan

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<tr>
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<th>Pressure</th>
<th>Pipe Reynolds Number</th>
<th>Solver</th>
<th>Radiation</th>
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</thead>
<tbody>
<tr>
<td>Pipe (1 m)</td>
<td>1.01 bar</td>
<td>1000</td>
<td>2d / 3d</td>
<td>P-1 / DO</td>
</tr>
</tbody>
</table>
Geometry and Temperature Boundary Condition for Test Case

CO₂
p = 1 atm
Re = 1000
T = 1200 K

1000 mm
1400 K

100 mm

CO₂
p = 1 atm
Re = 1000
T = 1200 K

1000 mm
1400 K
1000 K
1400 K
1000 K
Temperature Distribution for Different Radiation Models

P-1

DO
Temperature Distribution for Different Radiation Models

P-1

DO
Improved Results for HITECOM

- Radiation included via DO
- Incompressible ideal gas
- Gravity included

Simulation plan

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Temperature Distribution
Comparison Temperature Distribution with First Results
Summary

• First CFD studies provide fundamental knowledge of gas flow and temperature distribution inside the HITECOM reactor.
• The thermal boundary conditions influence significantly the thermal convection and hence the temperature and velocity distribution inside the reactor.
• The gas flow and temperature distribution in the vicinity of the boundary layer of the isolated particle are not constant, but allows for the investigation of isolate particles with a limited falsification due to wall effects.
Outlook

• Based on new data of the reactors structure, the temperature boundary conditions will be adjusted via UDFs.
• As a next step, isolated reacting particles, particle fixing and reacting gas flow will be implemented in the CFD model, in order to study the interaction between gas flow and particle inside the HITECOM reactor.
• Based on experimental data, existing particle-resolved CFD models will be validated intensively.