CFD simulation of 20 MW th CCL pilot plant reactors

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Motivation

Advantages of CFD tools

- Generation of numerical results within reasonable time → high computational cluster Lichtenberg

- Very flexible and well developed software tools e.g. Ansys Fluent™, OPEN FOAM → Implementation of customized models using UDFs

- Geometrical design studies quicker and more economic in comparison to experiments

- No expensive measurement technology required

Challenges for multiphase flows

- Complex interaction between fluid and particle phase

- Implementation of realistic sorbent properties → modeling approaches or experimental sample data required

- Compromise between accuracy and computational time
Applied modeling approaches

Overview of numerical methods

- Euler-Lagrange
  - Stochastic collision detection
    - MPIC (Barracuda, FLUENT)
  - Deterministic collision detection
    - DEM (FLUENT, DEMEST, OpenFoam)

- Euler-Euler
  - Kinetic theory of granular flows
    - Multi-Fluid model (FLUENT, CERTH)
CFD simulation of 20 MW$_{th}$ circulating fluidized bed carbonator using the coarse grain discrete element method

Alexander Stroh (Technische Universität Darmstadt)

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Outline

- DEM Modeling
- 20 MW\textsubscript{th} carbonator results
- Conclusion
DEM Modeling

Collision modeling

Normal force: \[ F^n = (k \delta + \gamma(v_{ij} \cdot n_{ij})) n_{ji} \]

\[ F^n \]
Particle \( j \)
\[ F^n \]
Particle \( i \)

\[ \delta \]

\[ F^n \rightarrow \bullet \rightarrow F^n \]
Dashpot

\[ F^n \rightarrow \bullet \rightarrow F^n \]
Spring

Tangential force: \[ F^t = F^n \mu \]

\[ \mu = f(v_{ij}) \] of collision partner

Cold flow experiments

Spouting bed regime

Bubbling bed regime
DEM Modeling

Particle modeling

1) Multicomponent particle
2) Ash particle

Ash particle is not participating in gas-solid reaction
1. Verification  →  2. Validation with experiments  →  3. Scale-up to 20 MW\textsubscript{th}

Charitos et al. for $X_{\text{MAX}} = 0.15 = \text{const.}$

\[
\frac{dX}{dt} = k_s S_0 (X_{\text{max}} - X)^2 (C_{CO_2} - C_{CO_2, eq})
\]

- Analytical
- CFD

- $C_{CO_2} - C_{CO_2, eq} \approx 1.179 \text{ mol/m}^3$
- $C_{CO_2} - C_{CO_2, eq} \approx 0.512 \text{ mol/m}^3$
- $C_{CO_2} - C_{CO_2, eq} \approx 0.220 \text{ mol/m}^3$
1. Verification → 2. Validation with experiments → 3. Scale-up to 20 MW\textsubscript{th}

DEM Modeling

Cold flow model

- 3.1 m
- 1.57 m
- 0.49 m

Graphs showing particle velocity vs. radial position.
DEM Modeling

1. Verification → 2. Validation with experiments → 3. Scale-up to 20 MWth

Gas concentrations at reactor outlet

<table>
<thead>
<tr>
<th></th>
<th>Exp.</th>
<th>Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>2.2</td>
<td>2.3</td>
</tr>
<tr>
<td>O₂</td>
<td>9.3</td>
<td>9.8</td>
</tr>
<tr>
<td>N₂</td>
<td>80.9</td>
<td>80.6</td>
</tr>
<tr>
<td>H₂O</td>
<td>7.2</td>
<td>7.4</td>
</tr>
</tbody>
</table>
DEM Modeling

1. Verification → 2. Validation with experiments → 3. Scale-up to 20 MW<sub>th</sub>

319,385 structured cells
orthogonal cell quality > 0.928

### Surface

<table>
<thead>
<tr>
<th></th>
<th>CFD boundary description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>distributor</td>
</tr>
<tr>
<td>2</td>
<td>from internal circulation</td>
</tr>
<tr>
<td>3</td>
<td>outlet</td>
</tr>
<tr>
<td>4</td>
<td>from calciner</td>
</tr>
<tr>
<td>5</td>
<td>Sorbent staging port 1</td>
</tr>
<tr>
<td>6</td>
<td>Sorbent staging port 2</td>
</tr>
</tbody>
</table>
20 MW\textsubscript{th} carbonator results

Pressure & solids distribution

\begin{align*}
\text{Pressure} & \quad \text{solids/m}^3 \\
\text{1000 kg/m}^2 & \quad 0.30 \\
\text{800 kg/m}^2 & \quad 0.28 \\
\end{align*}

\begin{align*}
\text{CO}_2 \text{ mass fraction} & \quad \text{kg CO}_2 / \text{kg Gas} \\
\text{1000 kg/m}^2 & \quad 0.16 \\
\text{800 kg/m}^2 & \quad 0.15 \\
\end{align*}
20 MW\textsubscript{th} carbonator results

**CO\textsubscript{2} mass fraction along reactor center axis**

- 1000 kg/m\textsuperscript{2}
- 800 kg/m\textsuperscript{2}

**CO\textsubscript{2} concentration along reactor cross sections**

- 1000 kg/m\textsuperscript{2}
- 800 kg/m\textsuperscript{2}

\[ \eta\text{\textsubscript{absorb}} \approx 88\% \]
Conclusion

- Developed coarse grain CFD-DEM model successfully verified and validated with experimental data
- Two numerical cases investigated with 1000 kg/m² and 800 kg/m² specific inventory for 20 MW\textsubscript{th}
  - solid concentration directly influences CO\textsubscript{2} capture
  - Carbonator absorption efficiency approximately 88 % for both specific inventories
- Reasonable computational time of ~ 30 days for industrial scale size unit using 32 parallel CPUs
Thank you for your attention!

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