CFD simulation of 1 MW<sub>th</sub> Carbonator using DDPM-DEM model

6<sup>th</sup> High Temperature Solid Looping Cycles Network Meeting

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SCARLET Consortium
Outline

- **Introduction**
  - Carbonate-Looping-Process
  - Discrete element method (DEM) model
  - Experimental & numerical boundary conditions

- **Results & model validation**
  - Influence of parcels number
  - Drag-models and bed inventory on time averaged pressure profile along reactor axis
  - Carbonation reaction implementation

- **Outlook**
Carbonate-Looping-Process

Carbonator

\[ T = 650 \, ^\circ \text{C} \]

\( \text{CO}_2 \)-lean flue gas

\( \text{CaCO}_3 \)

Calciner

\[ T = 900 \, ^\circ \text{C} \]

\( \text{CO}_2 \)

Flue gas

\( \text{CaO} \)

Make-up

Fuel

Ash

\( \text{O}_2 \)
DDPM-DEM model description

Collision modelling of DDPM-DEM approach

- DDPM can be used for any granular flow (e.g. fluidized bed, hoppers, pneumatic solid transport applications)

- Explicit particle tracking using Discrete Element Method (DEM) based on the Euler-Lagrange approach

- Soft-sphere contact model resolve particle-particle collisions

- Computational expensive for more than 500,000 particle parcels and small particle step size

Model simplification

- Particles are represented by spherical parcels

- Parcel collisions account for several particles with specific mass and volume

- Collision force laws (spring, spring-dashpot, friction)
Experimental & numerical boundary conditions

Temperature and Inventory assumed to be constant during steady-state operation

<table>
<thead>
<tr>
<th>Isothermal Temperature</th>
<th>908 [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inventory</td>
<td>220, 240, 260, 280 [kg]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mass flow (kg/s)</th>
<th>Species</th>
<th>Boundary</th>
<th>Boundary type</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.210528</td>
<td>Air</td>
<td>Air + CO2 inlet</td>
<td>Mass flow inlet</td>
</tr>
<tr>
<td>0.039994</td>
<td>Carbon dioxide</td>
<td>Air + CO2 inlet</td>
<td>Mass flow inlet</td>
</tr>
<tr>
<td>0.009722</td>
<td>Air</td>
<td>Solid inlet</td>
<td>Mass flow inlet</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>Outlet</td>
<td>Pressure outlet</td>
</tr>
</tbody>
</table>
**Ansys DDPM-DEM modeling**

**Assumption bed mass constant over time**

→ Particle injection implemented through User-Defined-Function

<table>
<thead>
<tr>
<th>Assumptions</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parcel number</td>
<td>$N_{\text{parc}} &gt; 200,000$</td>
</tr>
<tr>
<td>Parcel diameter</td>
<td>$d_{\text{parc}} &lt; 0.0116 \text{ m}$</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>$d_p = 91 \mu\text{m}$</td>
</tr>
<tr>
<td>Drag models</td>
<td>Syamlal O’Brien, Gidaspow, Gibilaro, Wen &amp; Yu, EMMS</td>
</tr>
<tr>
<td>DEM collision model</td>
<td>Spring dashpot for normal forces &amp; friction-dshf model for tangential forces</td>
</tr>
</tbody>
</table>

1. Determine bed inventory in each time step?
2. Inject particles through surface injection using `DEFINE_DPM_INJECTION_INIT` macro

<table>
<thead>
<tr>
<th>Numerical mesh investigation</th>
<th>structured coarse grid with 31,207 cells &amp; fine unstructured grid with 91,031 cells</th>
</tr>
</thead>
</table>
Ansys DDPM-DEM modeling
influence of bed inventory

Syamlal O'Brien drag model

- 220 kg solid inventory
- 240 kg solid inventory
- 260 kg solid inventory

Increasing solid flux

Increasing inventory

Solid mass flow rate (kg/s)

Pressure (Pa)

0.0 1000 2000 3000 4000 5000 6000 7000 8000 9000 10000 11000 12000

0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0

220 kg solid inventory
240 kg solid inventory
260 kg solid inventory

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influence of drag models

Drag models comparison using 220 kg of bed inventory

- Syamlal O'Brien
- WEN & YU
- Gidaspow
- Gibilaro
- EMMS [1]

Drag overprediction

0.0 1000 2000 3000 4000 5000 6000 7000 8000 9000
Pressure (Pa)

0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5
Height (m)
Ansys DDPM-DEM modeling influence of parcels number

Pressure profile along carbonator axis

- Experiment
- EMMS 300,000 parcels
- Gidaspow 200,000 parcels
- Gidaspow 300,000 parcels
- Gidaspow 500,000 parcels

Height (m) vs. Pressure (Pa)
Ansys DDPM-DEM reaction modeling

Applied reaction rate expression according Romano [2]

\[
\frac{dX}{dt} = k_s S_n (1 - X)^{2/3} \left( C_{\text{CO}_2} - C_{\text{CO}_2,eq} \right) \quad \text{with} \quad S_n = \frac{V_{\text{MCaCO}_3} X_{\text{Max}} \rho_{\text{CaO}}}{M_{\text{CaOH}}}
\]

intrinsic rate constant

specific available surface area

According Charitos et al. [3]

\[
\frac{dX}{dt} = k_s S_0 (X_{\text{Max}} - X)^{2/3} \left( C_{\text{CO}_2} - C_{\text{CO}_2,eq} \right)
\]

Applied constants from Abanades et al. [2,4]

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k_s) (m⁴/smol)</td>
<td>6.05*10⁻¹⁰</td>
</tr>
<tr>
<td>(V_{\text{MCaCO}_3}) (m³/mol)</td>
<td>36.9*10⁻⁶</td>
</tr>
<tr>
<td>(\rho_{\text{CaO}}) (kg/m³)</td>
<td>3320</td>
</tr>
<tr>
<td>(h) (m)</td>
<td>50*10⁻⁹</td>
</tr>
</tbody>
</table>
Ansys DDPM-DEM reaction modeling

Comparison of reaction rates Romano & Charitos

\[ C_{CO_2} - C_{CO_2eq} \approx 0.220 \text{ mol/m}^3 \]

\[ X_{\text{MAX}} = 0.10 \]

Charitos
Romano
Ansys DDPM-DEM reaction modeling

Single particle experiment

- Injected parcel with 0.009 kg
- Particle velocity set to zero through UDF
- Gas inlet velocity 10 m/s
- Different CO₂/N₂ concentrations

→ Recording carbonation degree over time in order to validate reaction model
Charitos et al. for $X_{\text{MAX}} = 0.15 = \text{const.}$

- $C_{\text{CO}_2} - C_{\text{CO}_2\text{eq}} \approx 1.179 \text{ mol/m}^3$
- $C_{\text{CO}_2} - C_{\text{CO}_2\text{eq}} \approx 0.512 \text{ mol/m}^3$
- $C_{\text{CO}_2} - C_{\text{CO}_2\text{eq}} \approx 0.220 \text{ mol/m}^3$

increased CO$_2$ concentration
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CO$_2$ concentration at Carbonator outlet

Relative deviation of mean values $\sim$ 10%

Simulation

Mean value from Experiment
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- Local particle velocities > 4 m/s

- dense region underpredicted with conventional drag models

- CO₂ gas concentration locally different

- at the outlet ~3 % [kg CO₂/kg Gas] (2.2 vol. %)

- CO₂ mainly captured in the bottom zone of Carbonator
Outlook

- Further 3-D model validation with new designed cold flow experiments
  - Improve implemented reaction model
  - Extend reaction model for particle size classes
  - Validation with pilot plant data for different experimental conditions

- Drag model development, implementation of filtered drag models in DDPM-DEM

- Sensitivity analysis (e.g. Bed inventory influence on capture efficiency, Make-Up Flow, PSD)

- Full-Loop simulation and experimental validation with 1MW\textsubscript{th} plant
Thank you for your attention.

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References


