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Modelling study of two chemical looping reforming reactor configurations: Looping vs. switching

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Modelling study of two Chemical Looping Reforming reactor configurations: Looping vs. Switching

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Outline

1. Objective
2. CLR vs. GSR principles
3. Simulations
4. Results and discussion
5. Conclusions
2. Objective of the work

To compare the performance of two pre-combustion reactor concepts

- Chemical Looping Reforming (CLR)
- Gas Switching Reforming (GSR)
### 3. CLR vs. GSR

<table>
<thead>
<tr>
<th><strong>CLR</strong></th>
<th><strong>GSR</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>• Two interconnected FBR reactors (AR and FR);</td>
<td>• One FBR for oxidation and reduction of the OC – <strong>switching concept</strong>;</td>
</tr>
<tr>
<td>• OC continuously transported between AR and FR;</td>
<td>• Alternating feed of air and fuel to the reactor unit;</td>
</tr>
<tr>
<td>• <strong>No mixing</strong> between N\textsubscript{2} and fuel;</td>
<td>• Undesired mixing between N\textsubscript{2} and fuel;</td>
</tr>
<tr>
<td>• Scale-up and operational challenges.</td>
<td>• <strong>Facilitates scaling-up</strong> under pressurized conditions.</td>
</tr>
</tbody>
</table>
4. Simulations

1-D phenomenological model for FBR

- **Generic formulation** based on the generic model developed by Abba et al. (2003)\(^1\);
- Uses an **averaging probabilistic approach** by Thompson et al. (1999)\(^2\);
- **Two-phase** model by Toomey and Johnstone (L- and H-phases) \(^3,4\);

### Differential Balances

- **Mass balance**
  - Gas total mass balance
  - Gas species mass balance for each phase
  - Total solids species mass balance
- **Total Energy balance**
- **Pressure Balance**

### Numerical scheme:

- Method of lines (MATLAB routine *ode15s*)
- Finite volume method (discretization in space)
  - Non-uniform grid
  - Convective term: 1\(^{st}\) order upwind scheme
  - Diffusion term: central differences scheme

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4. Simulations

Reactions and Kinetics

Reforming stage

Reforming\textsuperscript{[1]}

Ni as catalyst

\[ \text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2 \]

\[ \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \]

\[ \text{CH}_4 + 2\text{H}_2\text{O} \leftrightarrow \text{CO}_2 + 4\text{H}_2 \]

Fuel Reactor

Oxidation of the oxygen carrier\textsuperscript{[2]}

\[ \text{Ni} + \frac{1}{2} \text{O}_2 \leftrightarrow \text{NiO} \]

Oxidation stage

Reduction of the oxygen carrier\textsuperscript{[2]}

\[ \text{CH}_4 + 4\text{NiO} \leftrightarrow 4\text{Ni} + \text{CO}_2 + 2\text{H}_2\text{O} \]

\[ \text{H}_2 + \text{NiO} \leftrightarrow \text{Ni} + \text{H}_2\text{O} \]

\[ \text{CO} + \text{NiO} \leftrightarrow \text{CO}_2 + \text{Ni} \]

Reduction stage

Air Reactor


4. Simulations

**Simulation Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam flowrate</td>
<td>170 ton/h</td>
</tr>
<tr>
<td>Fuel flowrate</td>
<td>250 ton/h</td>
</tr>
<tr>
<td>Maximum temperature</td>
<td>1100 °C</td>
</tr>
<tr>
<td>Fuel inlet temperature</td>
<td>205 °C</td>
</tr>
<tr>
<td>Steam inlet temperature</td>
<td>400 °C</td>
</tr>
<tr>
<td>Operating pressure</td>
<td>17.3 bar</td>
</tr>
<tr>
<td>OC density</td>
<td>3446 kg/m3</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>250 µm</td>
</tr>
<tr>
<td>Reactor diameter</td>
<td>6 m</td>
</tr>
<tr>
<td>Reactor height</td>
<td>7 m</td>
</tr>
<tr>
<td>Axial resolution</td>
<td>20 cells</td>
</tr>
</tbody>
</table>

How to compare these two technologies?

Same simulation parameters and physical properties

Study variable: Degree of Oxygen Carrier utilization

How to adjust this parameter?
4. Simulations

**CLR: Oxygen carrier flux**

↓ OC flux: ↑ OC residence time

**GSR: Cycle time flux**

↑ cycle time: ↑ reduction + ↑ oxidation

Higher oxygen carrier conversion

<table>
<thead>
<tr>
<th>Degree of OC utilization (%)</th>
<th>CLR</th>
<th></th>
<th>GSR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>OC flux (kg/m² s)</td>
<td>Oxidation stage time (s)</td>
<td>Reduction stage time (s)</td>
</tr>
<tr>
<td>10</td>
<td>466</td>
<td>25</td>
<td>13</td>
</tr>
<tr>
<td>20</td>
<td>233</td>
<td>68</td>
<td>34</td>
</tr>
<tr>
<td>40</td>
<td>116.5</td>
<td>198</td>
<td>99</td>
</tr>
<tr>
<td>60</td>
<td>82.4</td>
<td>400</td>
<td>200</td>
</tr>
<tr>
<td>80</td>
<td>58.25</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
5. Results: Profiles

Chemical Looping Reforming: Fuel Reactor

- Reforming reactions dominate at the beginning of the reactor → system far from equilibrium conditions → production of H₂ → density decrease
- Reduction reactions dominate at the end;
- Low amount of NiO through the bed;
- Temperature almost constant → good axial mixing

Maximum values: 2.94 kg/m³ for the gas density, 1 for the void fraction, 2.4 m/s for the superficial velocity and 989 °C for the temperature
5. Results

Gas Switching Reforming

- O₂ totally consumed in the oxidation stage;
- Undesired mixture of N₂ with fuel → reduces CO₂ capture performance;

1. Oxidation
2. Reduction
3. Reforming
5. Results

Performance Measures

**CH$_4$ conversion**

**CO selectivity**

**H$_2$ production performance**

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**Higher OC utilization**

- Lower reduction temperature $\rightarrow$ low CH$_4$ conversion (by reforming endothermic reactions) $\rightarrow$ productivity of H$_2$ decreases
- Lower CO selectivity $\rightarrow$ WGS reaction

**Lower OC utilization**

- Lower CO selectivity $\rightarrow$ To supply heat

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**Higher OC utilization**

- Lower CH$_4$ conversion $\rightarrow$ Reforming stage is higher
- Lower H$_2$ productivity $\rightarrow$ lower CH$_4$ conversion

**Lower OC utilization**

- Higher amount of N$_2$ mixed with fuel $\rightarrow$ Short cycle times
6. Conclusions

1. CLR
   - Lower degree of OC utilization (higher OC circulation rate) → higher temperature in fuel reactor → better reforming performance
   - However, high OC circulation rate can bring practical and economic challenges

2. GSR
   - Lower degree of OC utilization (shorter stage times) → higher temperature in reforming stage → higher CH₄ conversion and H₂ production
   - However, undesired mixing of N₂ with CO₂ and syngas increases with shorter stage times
6. Conclusions

3. CLR vs. GSR

- H₂ production and CO conversion is higher in GSR
- Fuel conversion is higher for CLR with higher CO₂ content
- CLR is best suited to thermal power production with pre-combustion CO₂ capture and GSR to pure H₂ production
Thank you for your Patience!!!