A novel raw gas cooling system based on a CO conversion quench reactor
Outline

- Background and motivation
  - classic syngas production from coal
  - integrated CO quench conversion syngas production

- CO conversion quench reactor concept

- Modeling and results of simulation
  - CFD simulation
  - flowsheet simulation
  - thermochemical simulation

- Conclusions
Background and motivation

Classic syngas production from coal (for chemical syntheses)

- **Oxygen** → **Fuel** → **Entrained flow gasifier**
- **Rawgas + slag** → **Full water quench**
- **Quench gas 1** → **Scrubber**
- **Catal. CO conversion** → **CO₂/H₂S removal** → **Synthesis**
  - **Water-gas shift reaction:** \( CO + H₂O \leftrightarrow CO₂ + H₂ \)
  - **Syngas module:** \( M = \frac{X_{H₂} - X_{CO₂}}{X_{CO} + X_{CO₂}} \)
    - **3 % CO conversion**
    - **Advanced quench design forcing CO conversion**
Background and motivation

Integrated CO conversion syngas production

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Background and motivation

Integrated CO conversion syngas production

feed water (water bath)

raw gas + slag

entained flow gasifier

full water quench

oxygen fuel

quench gas1

T=216 °C

water+ slag (solid)

scrubber

bypass gas

synthesis

chemical product

CO2 H2S

M = 2.05 – 3.05

CO2/H2S removal

synthesis gas

fuel oxygen

HP water

HP steam

(water bath)

(catal. CO conversion)

(bypass gas)

M = 2.05 – 3.05

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Integrated CO conversion syngas production

Background and motivation

CO conversion quench

steam generator

scrubber
catal. CO conversion

CO₂/H₂S removal

synthesis

chemical product

M = 2.05 – 3.05
Optimized quench design

CO conversion quench reactor concept

- steam injection
  - keep the high temperature level
  - next to syngas inlet

- no built-in components
  - reduced slagging problems
  - optional water injection (below water line)

- residence time regulation
  - variable water bath fluid level

Parameter study

- detailed modelling and simulation (GriMech 3.0)
- three raw gases
- variation of steam temperature and mass flow

Results

- CO conversion rates up to 27 %
- characteristic CO conversion rate progression
- high gas outlet temperatures up to 1293 °C

H₂/CO ratio in terms of total H₂O/CO ratio

Example: reaction zone

**Example: reaction zone**

CFD result *)

model assumption

flowsheet model (detail)

reaction rate in kg $H_2/m^3s$

reaction zone

implementation in ASPENplus™

CO conversion quench reactor – flowsheet simulation

Model validation

- Inaccurate reproduction of CO conversion decrease at high steam mass flows

<table>
<thead>
<tr>
<th>Gas</th>
<th>Temperature</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas A</td>
<td>1450 °C</td>
<td>40 bar</td>
</tr>
<tr>
<td>gas B</td>
<td>1650 °C</td>
<td>40 bar</td>
</tr>
<tr>
<td>gas C</td>
<td>1500 °C</td>
<td>30 bar</td>
</tr>
</tbody>
</table>

- Small differences between gas outlet temperatures of CFD and flowsheet
CO conversion quench reactor – flowsheet simulation

Results: process chain

- **Catalytic CO conversion**
  - Design size decrease:
    - -8 % (Methanol)
    - -3 % (SNG)

- **Bypass gas ratio increase**:
  - 44 % to 51 % (Methanol)
  - 33 % to 38 % (SNG)

**Factsage™ model**

- **CO conversion quench**
  - T=900 °C
- **Steam generator**
  - T=260 °C
- **Scrubber**
- **Catal. CO conversion**
- **CO₂/H₂S removal**
- **Synthesis**

**M = 2.05 – 3.05**
### Results: fuel influence

<table>
<thead>
<tr>
<th>fuel</th>
<th>dried lignite</th>
<th>dried lignite + wood chips (49.1 wt.-%)</th>
<th>dried lignite + sewage sludge (8.2 wt.-%)</th>
<th>dried lignite + paper residue (2.6 wt.-%)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>alkali ash components (XRF analysis)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cl</td>
<td>wt.-%</td>
<td>0.24</td>
<td>0.23</td>
<td>0.18</td>
</tr>
<tr>
<td>K$_2$O</td>
<td>wt.-%</td>
<td>0.26</td>
<td>1.65</td>
<td>0.49</td>
</tr>
<tr>
<td>Na$_2$O</td>
<td>wt.-%</td>
<td>0.67</td>
<td>0.64</td>
<td>0.56</td>
</tr>
<tr>
<td><strong>volatile alkali raw gas components (calculated)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>KCl</td>
<td>bar</td>
<td>9.2 E-05</td>
<td>3.7 E-04</td>
<td>8.5 E-05</td>
</tr>
<tr>
<td>KOH</td>
<td>bar</td>
<td>1.8 E-05</td>
<td>1.3 E-04</td>
<td>1.8 E-05</td>
</tr>
<tr>
<td>NaCl</td>
<td>bar</td>
<td>3.4 E-05</td>
<td>2.6 E-05</td>
<td>2.6 E-05</td>
</tr>
</tbody>
</table>
Results: alkali condensation while raw gas cooling

- minor alkali separation by CO conversion quench process
- main alkali sink: steam generator
- below 500 °C heat exchanger less endangered

cooling below 500 °C by water injection
Conclusions

- validated flexible flowsheet model for the new CO conversion quench design
- balancing results demonstrate benefits of the new quench design
- slight contribution of alkali species to gas phase
- alkali deposition in convective gas cooling system requires adjustment of quench outlet temperature
THANK YOU FOR YOUR ATTENTION!

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