CFD Burner Study for Entrained Flow Gasifiers

Numerical Study of Different Burner Configurations in an Entrained Flow Gasifiers

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Motivation

Burner Development for Entrained Flow Gasification

State of the art
- Central jet flows
- Swirling and non-swirling jet flows
- 1 to 3 Distributed jet flows

Subjects of interest
- Increasing performance
- Shortened flame
- Stability of the flame
- Higher reaction rates

Bader et. al. 2018, Fuel Proc. Techn. 169

Motivation

Different Burner Concepts for Non-Catalytic Partial Oxidation of Natural Gas

Different burner concepts, Förster et. al. 2017, Fuel 203

Förster et. al. 2017, Fuel 203

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Outline

Burner Concepts Investigation for Entrained Flow Gasifiers

Fuel and Process Analysis for a Comprehensive CFD Model

Influence of the Burner Concept on the Reactor System

Conclusion and Outlook
Overview of the Reactor Design

Geometric boundary conditions

- Geometry of the reactor
- Geometry of the burners\(^1\)
  - Velocity profile of fuel inlet
  - Velocity profile of the oxidizer inlet
  - Velocity profile of the moderator inlet
  - Characteristics of the conveying system

- Entrained flow coal gasifier (top fired)
- Central jet burner
- 5.4 m high and \(\varnothing\) 2.3 m

\(^1\)Geometry influences the flow fields, Euler-Lagrange vs. real geometry
Burner Concepts Investigation for Entrained Flow Gasifiers

Burner Concepts (Inverse Models)

B1, central jet

B2, peripheral jet

B3, plate

B4, spherical

Siemens type reactor
Mesh

B1 and B2 central jets
- Dimension: 2D, axis-symmetric
- Size: 30k
- Type: structured, quadrilateral
- Calculation time: \( \sim 7 \) days

B3, plate
- Dimension: 3D, symmetry
- Size: 900k
- Type: structured, hexahedral
- Calculation time: \( \sim 50 \) days

B4, spherical
- Dimension: 3D, symmetry
- Size: 800k
- Type: structured, hexahedral
- Calculation time: \( \sim 50 \) days
## CFD Setup

Setup for the CFD setup of the Siemens type gasifier

<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>ANSYS Fluent</td>
</tr>
<tr>
<td>Turbulence</td>
<td>realizable $k$-$\varepsilon$ model</td>
</tr>
<tr>
<td>Radiation</td>
<td>DO model</td>
</tr>
<tr>
<td>Turbulence chemical interaction</td>
<td>Eddy-Dissipation Concept Model</td>
</tr>
<tr>
<td>Homogeneous mechanism</td>
<td>reduced GRI 1.2</td>
</tr>
<tr>
<td>Gas phase properties</td>
<td>kinetic theory</td>
</tr>
<tr>
<td>Particle tracking</td>
<td>Euler-Lagrange</td>
</tr>
</tbody>
</table>

Fuel and Process Analysis for a Comprehensive CFD Model

### Input Streams

#### Necessary operational boundary conditions

<table>
<thead>
<tr>
<th>Stream</th>
<th>Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal inlet</td>
<td>$m_{\text{coal}}, T_{\text{coal}}$</td>
</tr>
<tr>
<td>Oxidizer inlet</td>
<td>$m_{\text{ox}}, T_{\text{ox}}$</td>
</tr>
<tr>
<td>Moderator inlet</td>
<td>$m_{\text{mod}}, T_{\text{mod}}$</td>
</tr>
<tr>
<td>Purge inlet</td>
<td>$m_{\text{purge}}, T_{\text{purge}}$</td>
</tr>
<tr>
<td>Wall temperatures</td>
<td>$T_{\text{reactor}}, T_{\text{burner}}$</td>
</tr>
</tbody>
</table>

#### Boundary conditions criteria

<table>
<thead>
<tr>
<th>Condition</th>
<th>Criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min. gas temp.</td>
<td>$T_{\text{gas}} = T_{\text{crit-\eta}} + 50$ K</td>
</tr>
<tr>
<td>Fuel-oxygen-ratio</td>
<td>$\lambda = 0.4$ to $0.5$</td>
</tr>
<tr>
<td>Reactor pressure</td>
<td>$p_{\text{op}} = 31$ bar(a)</td>
</tr>
<tr>
<td>Carb. conv. target</td>
<td>$X_{\text{goal}} = \text{maximum}$</td>
</tr>
<tr>
<td>Thermal power</td>
<td>$\dot{H}_{\text{th}} \sim 250$ MW</td>
</tr>
<tr>
<td>Fuel HHV</td>
<td>$\Delta h_{\text{HHV,ar}} = \text{Newland hard coal}$</td>
</tr>
<tr>
<td>Conveying system</td>
<td>$\varepsilon_{\text{void}} \approx 0.75$</td>
</tr>
</tbody>
</table>

#### Remark
- Operational experience
- Equilibrium approach
- Non-equilibrium reduced order models
- Most reliable boundary conditions
### Input Streams Approximation for the Current Setup

#### General boundary conditions

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel stream</td>
<td></td>
</tr>
<tr>
<td>$m_{\text{coal}}$, kg/s</td>
<td>9.0</td>
</tr>
<tr>
<td>$m_{\text{CO}_2}$, kg/s</td>
<td>1.0</td>
</tr>
<tr>
<td>$T_{\text{purge}}$, K</td>
<td>300.0</td>
</tr>
<tr>
<td>Gasifying stream</td>
<td></td>
</tr>
<tr>
<td>$m_{\text{gas}}$, kg/s</td>
<td>7.5</td>
</tr>
<tr>
<td>$x_{\text{O}<em>2}$, $x</em>{\text{CO}_2}$</td>
<td>0.95, 0.05</td>
</tr>
<tr>
<td>$T_{\text{gas}}$, K</td>
<td>653.0</td>
</tr>
<tr>
<td>Wall inlet region</td>
<td></td>
</tr>
<tr>
<td>$T_{\text{burner}}$, K</td>
<td>300.0</td>
</tr>
<tr>
<td>Wall reactor</td>
<td></td>
</tr>
<tr>
<td>$T_{\text{reactor}}$, K</td>
<td>1600.0</td>
</tr>
<tr>
<td>Reactor pressure</td>
<td></td>
</tr>
<tr>
<td>$p_{\text{op}}$, bar(a)</td>
<td>31.0</td>
</tr>
</tbody>
</table>

Example of burner boundary conditions
Fuel and Process Analysis for a Comprehensive CFD Model

General Fuel Properties

**Standard analysis**
- Ultimate analysis
- Proximate analysis
- Intrinsic surface
- Density and porosity
- Higher heating value
- Particle size distribution
- Ash characteristics (e.g. temperature of critical viscosity)

**Advanced measurements of the used fuel**
- Pyrolysis rates and composition
- Heterogeneous reaction kinetics ($CO_2$ and $H_2O$)

**Remark** All data need to be available for the same fuel
Properties of the pyrolysis process

- Based on particle heating rates
  - Experimental determination as close to the operation conditions as possible
- Comprises
  1. Pyrolysis gas compositions and tar properties
  2. Devolatilization rates for all participating species
  3. Swelling index

- Goal is to use experimental data (e.g. PYMEQ rig)\(^1\)

- No data set for the desired coal is available
  - Use of network models is necessary

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\(^1\)Reichel et al. 2015, Fuel 158
Newland Coal

<table>
<thead>
<tr>
<th>Proximate analysis (ar), wt %</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>FC</td>
<td>55.6</td>
<td>27.8</td>
<td>13.4</td>
<td>3.2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ultimate analysis (daf), wt %</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>82.50</td>
<td>5.11</td>
<td>10.61</td>
<td>1.36</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Other properties</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (true), kg/m³</td>
<td>1456.0</td>
<td></td>
</tr>
<tr>
<td>HHV (ar), MJ/kg</td>
<td>28.88</td>
<td></td>
</tr>
</tbody>
</table>

1Kajitani et al. 2003, Report W02021
Results of the Chemical Percolation Model

Particle temperature over time (CPD vs. SFOM)

Particle temperature over time (CPD vs. C2SM)

Final mass fraction yield, wt.%

<table>
<thead>
<tr>
<th>Compound</th>
<th>Yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>12.00</td>
</tr>
<tr>
<td>CH₄</td>
<td>6.27</td>
</tr>
<tr>
<td>CO</td>
<td>5.40</td>
</tr>
<tr>
<td>CO₂</td>
<td>3.49</td>
</tr>
<tr>
<td>Tar</td>
<td>20.15</td>
</tr>
</tbody>
</table>

Final mass fraction yield, wt.%

Tar

C₁₃.₇H₂₁.₄N₁.₀₁

with \( M_{\text{tar}} = 200 \frac{\text{kg}}{\text{kmol}} \)

\[-\frac{dm_p}{dt} = k \cdot [m_p - (1 - f_{v,0})(1 - f_{w,0}) \cdot m_{p,0}] \quad \text{with} \quad k = A \cdot \exp \left(-\frac{E_A}{T \cdot R_u} \right)\]

with \( A = 13436655 \frac{1}{\text{s}} \) and \( E_A = 80970 \frac{\text{J}}{\text{mol}} \)

\[\text{Vol} \rightarrow 0.4659 \text{H}_2\text{O} + 0.2734 \text{CH}_4 + 0.1348 \text{CO} + 0.0555 \text{CO}_2 + 0.0705 \text{Tar}\]
Heterogeneous Reaction Kinetics

**Literature data**
- Reliability ↓
- Availability ↑
- mainly based on TGA measurements
- limited usability

**TGA**
- Fast
- Reliable
- Several systems available at the institute
- Experience in model based data evaluation
- Advantage in determining rate in kinetic controlled regime

**Drop tube**
- KIVAN
- Sophisticated and complex
- Closer to the real process
- Reliable for regime I + II
- Best kinetic data for entrained flow gasifiers

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2. Gonzalez et al. 2018, Fuel 224
4. ANSYS Fluent Manual v172, ch. 7.3

**Literature data** are adapted for surface based kinetics

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TU Bergakademie Freiberg | T. Förster et al. | CFD Burner Study for Entrained Flow Gasifiers | 18.05.2018
Influence of the Burner Concept on the Reactor System

Flow Fields, Velocity Magnitude, $v_{axial} = 0 \text{ m s}^{-1}$

B1, jet central  
B1, swirl 60°  
B3, plate  
B4, spherical
Influence of the Burner Concept on the Reactor System

Gas Residence Time

- B1, jet central
- B1, swirl 60°
- B3, plate
- B4, spherical
Influence of the Burner Concept on the Reactor System

Overall Particle Residence Times

B1, jet central

B1, swirl 60°

B3, plate

B4, spherical
Influence of the Burner Concept on the Reactor System

Heterogeneous Burnout, \( r_{C+O_2} = 0.1 \text{ kmol/m}^3\text{s} \)

- B1, jet central
- B1, swirl 60°
- B3, plate
- B4, spherical
Conclusion

- State of the art CFD models for detailed conversion analysis are available
- Different burner concepts including swirl were investigated for the prove of general concept
- The burner configuration has a great impact on flow and particle dynamics in a reactor
- Findings for single-phase systems cannot be transferred directly to multiphase systems.

Next steps

- Additional burner concepts will be studied
- Implementation of new fuel datasets based on in-house measurements
- Usage of ROMs for a better pre-assessment of boundary conditions for CFD
Thank you for your kind attention!

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