Two-Dimensional CFD Simulation for Industrial Coal-Water Slurry Entrained Flow Gasifier
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Content Outline

Motivation and Purpose

Coal Water Slurry Gasifier Modeling

Simulation Results and Discussions
  • Simulation Results
  • Influence of Turbulence – Chemistry Interaction Model
  • Non-reactive Cold and Reactive Flow Simulation Results
  • Influence of Operation Condition

Conclusions

Outlook
Motivation

- Coal is the major source of energy in China
  Chemical products from coal: CTG, CTL, CTM (MTO, MTA)
- Importance of gasification process
  Process stability, overall efficiency, investment
- Entrained flow gasification technology
  Advantages: high carbon conversion ratio, wide adaption to different types of coal, large production capacity
- Challenges in developing entrained flow gasification
  Fluctuate of coal qualities, scale up effect, harsh condition for experiment
- Comprehensive model for entrained flow gasification
  Optimization of gasifier design and operation condition
Purpose

- Developing comprehensive coal water slurry (CWS) entrained flow gasifier model
  - Evaporation, devolatilization, volatile decomposition, gas phase and char reactions
- Comparing turbulence – chemistry interaction models
  - FR/ED model, EDC model
- Analyzing simulated cold and reactive flow field
- Sensitivity analysis of operation conditions
  - Pressure, coal water slurry concentration, droplet size distribution
Coal Water Slurry Gasifier Modeling

- Gasification chamber geometry and mesh
  2D axial symmetry quadrilateral mesh
- Operation and boundary conditions

<table>
<thead>
<tr>
<th>Ultimate Analysis, wt%</th>
<th></th>
</tr>
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<tbody>
<tr>
<td>C, daf</td>
<td>79.72</td>
</tr>
<tr>
<td>H, daf</td>
<td>4.56</td>
</tr>
<tr>
<td>O, daf</td>
<td>14.64</td>
</tr>
<tr>
<td>N, daf</td>
<td>0.88</td>
</tr>
<tr>
<td>S, daf</td>
<td>0.20</td>
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</table>

<table>
<thead>
<tr>
<th>Proximate Analysis, wt%</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Volatile, dry</td>
<td>60.02</td>
</tr>
<tr>
<td>Fixed carbon, dry</td>
<td>33.23</td>
</tr>
<tr>
<td>Ash, dry</td>
<td>6.75</td>
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<table>
<thead>
<tr>
<th>Item</th>
<th>Settings</th>
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<tbody>
<tr>
<td>Operation pressure, MPa</td>
<td>4.0</td>
</tr>
<tr>
<td>CWS mass rate, kg/s</td>
<td>18.210</td>
</tr>
<tr>
<td>CWS temperature, K</td>
<td>333.15</td>
</tr>
<tr>
<td>Water volume fraction, %</td>
<td>50.53</td>
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<tr>
<td>Oxygen mass flow rate, kg/s</td>
<td>9.987</td>
</tr>
<tr>
<td>Oxygen temperature, K</td>
<td>313.15</td>
</tr>
<tr>
<td>Average droplet diameter, mm</td>
<td>0.188</td>
</tr>
</tbody>
</table>
Sub-models

- **Evaporation Model**

  Diffusion controlled model

  \[
  \frac{d m_p}{d t} = -A_p M_{w,l} k_c \left( \frac{p_{sat}(T_p)}{RT_p} - X_i \frac{p}{RT_{\infty}} \right)
  \]

  \[
  Sh_{AB} = \frac{k_c d_p}{D_{i,m}} = 2.0 + 0.6 \text{Re}_{d}^{1/2} \text{Sc}^{1/3}
  \]

- **Pyrolysis Model**
  - **Devolatilization**
    - Single kinetic step rate

  \[
  -\frac{d m_p}{d t} = k \left[ m_p - (1 - f_{v,0})(1 - f_{w,0})m_{p,0} \right]
  \]

  \[
  k = 3.82 \times 10^5 \exp \left( \frac{-7.4 \times 10^7}{RT} \right)
  \]

  - **Volatile Decomposition**

    \[
    Vol \rightarrow a_1CH_4 + a_2CO + a_3CO_2 + a_4H_2 + a_5N_2 + a_6H_2S + a_7H_2O
    \]

<table>
<thead>
<tr>
<th>T, K</th>
<th>P, MPa</th>
<th>Mw</th>
<th>a₁</th>
<th>a₂</th>
<th>a₃</th>
<th>a₄</th>
<th>a₅</th>
<th>a₆</th>
<th>a₇</th>
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<tbody>
<tr>
<td>1000</td>
<td>4.0</td>
<td>18.468</td>
<td>0.425</td>
<td>0.124</td>
<td>0.113</td>
<td>0.194</td>
<td>0.016</td>
<td>0.003</td>
<td>0.124</td>
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</table>

\[
R_{Vol} = 2.199 \times 10^{11} \exp \left( -\frac{2.027 \times 10^8}{RT} \right) C_{Vol}^{0.2}
\]
**Reaction Mechanism**

**Homogeneous Reaction**

\[ CO + 0.5O_2 \rightarrow CO_2 \]
\[ H_2 + 0.5O_2 \rightarrow H_2O \]
\[ CH_4 + 0.5O_2 \rightarrow CO + 2H_2 \]

\[ CO + H_2O \leftrightarrow CO_2 + H_2 \]
\[ CH_4 + H_2O \leftrightarrow CO + 3H_2 \]

**Char Reaction**

\[ C + 0.5O_2 \rightarrow CO \]
\[ C + CO_2 \rightarrow 2CO \]
\[ C + H_2O \rightarrow CO + H_2 \]

**Turbulence – chemistry interaction model**

**Finite Rate/ Eddy Dissipation**

\[ R_{i,r} = v'_{i,r} M_{w,i} A \rho \frac{\varepsilon}{k} \min_R \left( \frac{Y_R}{v'_{R,r} M_{w,R}} \right), \quad R_{i,r} = v'_{i,r} M_{w,i} A B \rho \frac{\varepsilon}{k} \sum_{j}^N \frac{Y_P}{v''_{j,r} M_{w,j}} \]

**Eddy Dissipation Concept**

\[ \gamma = \left( \frac{100 \frac{3C_{D2}}{4C_{D1}}^{1/4}}{\eta} \right), \quad \tau^* = \left( \frac{C_{D2}}{3} \right)^{1/2} \tau_\eta, \quad R_i = \frac{\rho \gamma^2}{\tau^* (1 - \gamma^3)} (Y_i - Y_i) \]
Results and Discussions

- Temperature distribution

- Streamline distribution
Gas concentration distribution
● Particle residence time distribution

- Comparison with process design data

<table>
<thead>
<tr>
<th>Mole fraction at outlet of gasification chamber, %</th>
<th>Xc, %</th>
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<tbody>
<tr>
<td>CO</td>
<td>H₂</td>
</tr>
<tr>
<td>Simulation</td>
<td>35.06</td>
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<tr>
<td>Design Data</td>
<td>33.8</td>
</tr>
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Influence of Turbulence – Chemistry Interaction

- Turbulence – Chemistry interaction

**Eddy Dissipation Model**

\[
R_{i,r} = \nu_{i,r} M_{w,i} A \rho \frac{\varepsilon}{k} \min_R \left( \frac{Y_R}{\nu_{R,r} M_{w,R}} \right), \quad R_{i,r} = \nu_{i,r} M_{w,i} AB \rho \frac{\varepsilon}{k} \sum_p Y_p
\]

**Eddy Dissipation Concept Model**

\[
\gamma = \left( \frac{100 C_D^2}{4 C_{D,1}^2} \right)^{1/4} \left( \frac{\eta}{\lambda} \right), \quad \tau^* = \left( \frac{C_D^2}{3} \right)^{1/2}, \quad \tau_{\eta}, R_i = \frac{\rho \tau^2}{\tau^* (1 - \gamma^3)} (Y_i - Y_i^*)
\]

- Comparison of ED and EDC models

[Diagram of temperature distribution with labels FR/ED and EDC]
<table>
<thead>
<tr>
<th></th>
<th>CO</th>
<th>H₂</th>
<th>CO₂</th>
<th>H₂O</th>
<th>Xc</th>
</tr>
</thead>
<tbody>
<tr>
<td>EDC Model</td>
<td>35.06</td>
<td>28.45</td>
<td>14.79</td>
<td>21.38</td>
<td>97.70</td>
</tr>
<tr>
<td>FR/ED Model</td>
<td>42.29</td>
<td>25.46</td>
<td>9.49</td>
<td>22.06</td>
<td>98.08</td>
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<tr>
<td>Design Data</td>
<td>33.8</td>
<td>27.3</td>
<td>16.2</td>
<td>22.2</td>
<td>97.16</td>
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Non-reactive Cold and Reactive Flow Simulation Results

- Comparison of streamline distribution

- Particle residence time distribution
Influence of Operation Condition

- Operation pressure (4MPa to 5MPa)
- Slurry concentration (49.5% to 47.1% vol)
Mean droplet diameter (188\(\mu\)m to 376\(\mu\)m)
Conclusions

- The comprehensive 2-D CFD model for industrial CWS gasifier is approved by process design data.
- Comparison of CFD results obtained by FR/ED and EDC are presented. The simulation results show that EDC model is more suitable for gasification simulation.
- Significant differences of streamline distribution and particle residence time distribution for cold and reactive flow simulation are observed. The jet-core region is elongated since gas releasing in reactive flow.
- Ascending operation pressure increases syngas yield, and low slurry concentration leads to less CO concentration and higher H$_2$/CO ratio. The coarse particle results in lower syngas concentration and carbon conversion ratio.
Outlook

- Specifying volatile decomposition and char reaction kinetic parameters based on experiment data.
- Implementing sensitivity analysis of sub-models including turbulence, evaporation, devolatilization and volatile decomposition models, and mesh independent check.
- Comparison of 2D and 3D CFD models of gasification chamber.
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Thank you for your attention

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