CFD simulation of pulverized fuel combustion, gasification and ash deposition in entrained flow reactors

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Outline

• Motivation

• **Part I: Gasification kinetics**
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  • Experimental facilities
  • Meshing
  • Solution strategy
  • Results

• **Part II: Ash deposition**
  • Deposition mechanisms
  • Experimental setup
  • Mathematical model
  • Validation

• Summary and Outlook
Motivation

Classification of gasifier types:

<table>
<thead>
<tr>
<th></th>
<th>Fixed bed</th>
<th>Fluidized bed</th>
<th>Entrained flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet temperature</td>
<td>425-600 °C</td>
<td>900-1050 °C</td>
<td>1250-1600 °C</td>
</tr>
<tr>
<td>Oxidant demand</td>
<td>Low</td>
<td>Moderate</td>
<td>High</td>
</tr>
<tr>
<td>Ash conditions</td>
<td>Dry ash or slagging</td>
<td>Dry ash or agglomerating</td>
<td>Slagging</td>
</tr>
<tr>
<td>Size of coal feed</td>
<td>6-50 mm</td>
<td>6-10 mm</td>
<td>&lt; 100 µm</td>
</tr>
<tr>
<td>Acceptability of fines</td>
<td>Limited</td>
<td>Good</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Other characteristics</td>
<td>Methane, tars and oils present in syngas</td>
<td>Low carbon conversion</td>
<td>Pure syngas, high carbon conversion</td>
</tr>
</tbody>
</table>
Motivation

Aims and purposes of the simulation:

• Prediction of carbon conversion and product gas composition at conditions relevant to industrial scale gasifier operation (high pressures and temperatures)

• Optimization of the gasification process and the gasifier design with focus on fuel flexibility (biomass and coal)

• Prediction of ash deposition
Motivation

Why CFD?

• Calculation of complex geometries (e.g. industrial scale gasifier)
• Taking into account turbulence models and particle tracks
• Taking into account particle radiation and particle size distribution
• Implementation of particle deposition and slagging model is possible
• Visualization of the results help to better understand the gasification process
Part I

Gasification kinetics
Modeling of the gasification process

Gasification:

“A process that uses heat, pressure and steam to convert materials directly into a gas composed primarily of carbon monoxide and hydrogen.”

Key steps in a gasification process:

- Drying
- Volatile release
- Homogeneous and heterogeneous reactions
Modeling of the gasification process

Heterogeneous reactions:

R1 (C oxidation): $C + 0.5O_2 = CO$
R2 (Boudouard): $C + CO_2 = 2CO$
R3 (Reforming): $C + H_2O = CO + H_2$

Homogeneous reactions:

R4 (Volatile oxidation): $C_{x_1}H_{x_2}O_{x_3}N_{x_4} + \left(\frac{x_1-x_3}{2}\right)O_2 = x_1CO + \frac{x_2}{2}H_2 + \frac{x_4}{2}N_2$
R5 (H$_2$ oxidation): $H_2 + 0.5O_2 = H_2O$
R6 (CO oxidation): $CO + 0.5O_2 = CO_2$
R7 (WGS): $CO + H_2O \leftrightarrow CO_2 + H_2$
Modeling of the gasification process

- **Regime I**: At low temperatures the intrinsic rate is slower than pore and bulk diffusion

- **Regime II**: The pore diffusion cannot keep up with the chemical reaction rate at increased temperatures

- **Regime III**: At high temperatures the bulk diffusion limits the overall reaction rate

\[
r = r(T, p_i, K_i, ...) \quad \left[ \frac{g}{g \cdot s} \right]
\]
Modeling of the gasification process

\[ R_{i,I} = A_t \cdot k_i \cdot p_{S,i}^n, \quad p_{S,i} = p_{\text{bulk}} \]

\[ R_{i,II} = \eta_i \cdot A_t \cdot k_i \cdot p_{S,i}^n \]

\[ R_{i,III} = \frac{12 \cdot N_i \cdot D_{M,i} \cdot M_i}{d_p^2 \cdot \rho_p \cdot R \cdot T_{\text{bulk}}} \cdot \left( p_{\text{bulk}} - p_{S,i} \right)^0 \]

C+CO\(_2\), \( p=1\text{bar} \), 30\% partial pressure CO\(_2\), \( d_p=120\mu\text{m} \), \( \rho_p=1400\text{kg/m}^3 \), Tortuosity = 3, \( A_{t_0} = 230 \text{ m}^2/\text{g} \)
Experimental facilities

- Atmospheric and pressurized entrained flow reactor
- Possible operation with $\text{N}_2$, $\text{O}_2$, $\text{H}_2$, $\text{CO}_2$, $\text{H}_2\text{O}$, Ar, CO
- Maximum temperature = 1800 ºC
- Maximum pressure = 50 bar
Solution strategy – Journal file

- **100 Iterations**
  - Calculation of the fluid flow with k-ε turbulence model
  - First order discretization

- **200 Iterations**
  - Including the energy equation and the radiation model (Discrete Ordinates)

- **100 Iterations**
  - Second order discretization

- **ca. 2000 Iterations**
  - Including species transport, reactions (FR-EDM) and particles (DPM, Lagrange)
  - Adjusting the under relaxation factors
Results – Stability and convergence

![Graph 1: Convergence history of Static Temperature on outlet](#)

![Graph 2: Scaled Residuals](#)

![Graph 3: Convergence history of Mass fraction of co on outlet](#)

![Graph 4: Convergence history of Mass fraction of h2 on outlet](#)
Results – Gas composition

CO      CO₂      H₂       H₂O      N₂       O₂   Volatiles

Reaction rate [kmol/(m³ s)]

z [m]  RR1 [kmol/(m³ s)]  RR2 [kmol/(m³ s)]  RR3 [kmol/(m³ s)]  RR4 [kmol/(m³ s)]  RR5 [kmol/(m³ s)]  RR6 [kmol/(m³ s)]  RR7 [kmol/(m³ s)]  RR8 [kmol/(m³ s)]  RR9 [kmol/(m³ s)]

z [m]  0,002  0,004  0,006  0,008  0,01  0,012  0,014  0,016  0,018

Mole fraction [\text{-}]

z [m]  CO [-]  CO₂ [-]  H₂ [-]  H₂O [-]  N₂ [-]  O₂ [-]  Vol [-]

z [m]  0  0,002  0,004  0,006  0,008  0,01  0,012  0,014  0,016  0,018
Results – Mean values
Part II

Ash deposition
Deposition mechanisms

• **Mechanisms building depositions:**
  - Inertial impaction
  - Condensation
  - Thermophoresis
  - Chemical reactions (heterogeneous reactions with deposits)

• **Mechanisms removing depositions:**
  - Erosion (by sharp unmolten particles impacting with high mass and velocity)
  - Shedding (by gravity and weak strength)
  - Shedding (by thermally or mechanically induced stresses)
  - Melting and drip off
Experimental setup

• **Entrained flow reactor**
  - Electrically heated (up to 50 kW<sub>el</sub>)
  - Fuels up to 2 kg/h (or 15 kW<sub>th</sub>)

• **Investigations on different solid fuels under varying conditions:**
  - Temperatures (up to 1600 °C)
  - Air-fuel ratio (oxidizing or reducing)
  - Fuels (bit. coal, lignite, biomass)
  - (Oxidation medium)
Mathematical model – deposition growth

- Calculation of stationary deposition rates (sticking criterion based on TGA/DTA measurements)
- Calculation of deposit layer thickness $dx$ for each cell
- Identification of cell nodes
- Grid modification for each cell node and adjacent cells
- Adjust thermal conductivity of underlying cell
- Iteration of fluid flow until new stationary solution with changed deposition rate and surface temperatures

$$dx = \frac{\phi_{dep} \cdot t}{\rho_{solid} \cdot (1 - \varepsilon)}$$
Mathematical model – Turbulent Dispersion

Particle trajectory is calculated by including an instantaneous value of the flow velocity (RANS-equations).

- Turbulent kinetic energy is used to calculate statistical particle trajectory
- Strong influence on particle tracks
- There are two different models available in literature: Cloud Model, Discrete Random Walk Model
Comparison of experimental results and predictions

Deposition rates [mm/h]:

Deposition photographs:
Comparison of experimental results and predictions

Prediction of deposit growth over time:

Deposit layer thickness [mm]

Flow direction

t = 0.00h

Flow direction

t = 1.25h

Flow direction

t = 2.50h
Summary

• Prediction of char conversion, gas composition and ash deposition
• Detailed modeling of heterogeneous reaction rates by means of a User Defined Function (DEFINE_PR_RATE), including several sub-models
• Good convergence by applying a journal-file-based solution strategy
• Mathematical model is able to capture deposition process and growth
• Particle diameter and deposit porosity are crucial parameters
Outlook

• Intrinsic reaction rates are needed as input parameters for each biomass or coal, in order to validate the CFD model with the lab-scale gasifiers at the Institute

• Further development of the particle reaction model:
  • More detailed devolatilization approach
  • Temperature-dependent $d/\rho$ evolution (burning mode)
  • Detailed kinetics of WGS reaction kinetics by means of a UDF

• Particle diameter and density evolution (fragmentation, condensation)

• Validation for different parameters (temperature and air-fuel ratio), fuels
Thank you for your attention!