Numerical Simulation of Biomass Gasification in a Steam-Blown Bubbling Fluidized Bed


Department of Mechanical Engineering
Massachusetts Institute of Technology

NETL Workshop of Multiphase Simulations, August 12-13, 2015

Project support by BP
Steam-blown fluidized bed gasifiers

**Fluidized bed:** Favorable reactor technology for biomass gasification with minimum pretreatment

**Advantages:**
- High levels of intermixing
- Suitable for coarse particles with large residence times

**Disadvantages:**
- Lower levels of carbon conversion with considerable tar content

**Steam as a gasification agent:**

**Advantages:**
- Reduced cost, no air separation is needed
- In the absence of oxidation, hot zones are avoided in the bed

**Disadvantages:**
- Biomass devolatilization and char gasification are endothermic
- External heating is needed for controlling the process
Key phenomena in a fluidized bed gasifier

Multi-scale process:
- Gas-phase chemistry
- Surface chemistry
- Single-particle modeling
- Hydrodynamics

Goal
- Development of a multiscale CFD methodology for the reactive multiphase simulations to assist the design and optimization of gasification processes by reducing the cost, compared with experiments, and offering information for integration in ROM
Modeling Challenges: Initial char loading

- **Challenge:** Steady state char inventory takes hours to reach for gasification conditions
  - Initial transient too long for CFD simulation
- **Solution:** Standalone MATLAB steady state char conversion model computes char inventory for CFD initial condition
  - Char gasification and combustion
  - Gasification assisted attrition due to hardness reduction
Steady state char inventory for steam blown gasifier

Gas composition (XCO2, XH2O...)
Reactor temperature, pressure,
Initial biomass particle size

Inputs:

Char conversion model
\( \dot{m}_{\text{in, raw}} [kg/sec] \) steady biomass feed rate
\( Y_{\text{char}} [kg/kg] \) char devolatilization yield

Transient model:
System of ordinary differential equations

Steady state model:
Iterative solver for average residence time

Outputs:
Average char inventory (kg)
Average char resident time (sec)
Average char conversion (-)

Computational cost <1 sec

CFD initial conditions:
- char inventory
- particle size

T=700 °C

\( H_{\text{char}} = 24.8 \text{ cm} \)
\( d_{\text{reactor}} = 10.2 \text{ cm} \)
\( m_{\text{char}} = 138 \text{ g} \)
\( V_{\text{char}} = 2029 \text{ cm}^3 \)
Modeling Challenges: Chemistry description

- **Challenge:** Number of species/reactions prohibitively large for use in CFD
- **Solution:** Use of Global models for pyrolysis and tar cracking [1]
Global devolatilization model

• Devolatilization dynamics are strongly influenced by particle radius.
• Shrinking Core Model Implemented for Eulerian Modeling Framework:

\[ k_{eff} = \frac{1}{k_{kin}} + \frac{a}{k_{cond}} \]

• Trade-off of devolatilization time and mixing time important for well-stirred assumption.
Modeling Challenges: Hydrodynamics

- Raw biomass injected as particles and removed as char
- Biomass typically <2-3% of bed mass
- Bed temperature 600-1000°C
- Very rapid heat up
- **Mixing and particle residence times** are very important to product composition and conversion

Devolatilization time scales are similar with mixing time scales, so accurate prediction of the position of raw biomass is important.
CFD modeling strategy for gas-particle flows

**Two Fluid Model**

Both phases are considered as fully interpenetrating continua

- Gas Phase → Eulerian Framework
- Particle Phase → Eulerian Framework

**ADVANTAGE:** High computational efficiency makes this method more attractive since parametric and design studies of large-scale systems are feasible

**DISADVANTAGE:** Closures are required for the modeling of:
- Interphase momentum exchange
- Particle-particle interaction

Numerical tool: **MFIX (DOE-NETL)** [2,3]
## NREL gasifier

### Experimental Parameter | Value
---|---
**Bed material**
Size, \( d_p \),
Density \( \rho_p \) | Olivine \((\text{Mg,Fe})_2\text{SiO}_4\)
270 \( \mu \text{m} \)
3300 kg/m\(^3\)

**Minimum Fluidization** \( u_{mf} \) | \( \sim 0.037 \text{m/s} \)

**Superficial velocity**, \( u_0 \) | \( \sim 0.12 \text{ m/s} \)

**Bed diameter**, \( d_{bed} \)
**Bed Height** | 4”(0.106 m),
0.13 m

**Bed temperature**, \( T_{bed} \)
(heated walls) | 750, 800, 850 \( \degree \text{C} \),

**Inlet gas composition** \( X_{feed} \) | 100% H\(_2\)O(%vol)
<2% Helium

**Input biomass feed rate** \( \text{bio,0} \) | 800g/hour

**Biomass mean diameter** \( d_{bio,0} \) | 1 mm

**Steam flow rate** | 800g/hour

---

![Diagram of NREL gasifier](image-url)
Simulation setup

- 2D simulations of a steam blown gasifier (Both reacting and non-reacting)
- 3 solid phases considered
  - Biomass: \( \text{Rho}=600 \text{kg/m}^3, d=1 \text{mm} \)
  - Char: \( \text{Rho}=170 \text{kg/m}^3, d=0.38 \text{mm} \)
  - Sand: \( \text{Rho}=3300 \text{kg/m}^3, d=0.27 \text{mm} \)
- Drag model: Gidaspow
  - Friction coefficient, \( C_f = 0.1 \)
  - Segregation slope coefficient, \( C_s = 0.1 \)
- Partial slip BC for solids
- Specularity coefficient, \( \phi = 0.05 \) [5,6]
- Dirichlet BC for temperature (1023 K) along walls and inflow
- Initial Condition
  - Static bed height: 24.4 cm
  - \( \varepsilon_{s,\text{sand}} = 0.4582 \)
  - \( E_{s,\text{char}} = 0.1218 \)
- Resolution: 40X400 cells
Chemistry description

Chemical mechanism

• Drying

• Devolatilization (Competing pathways following Gronli 2000 [7])

  \[ \text{bio} \rightarrow 7.7872\text{H}_2 + 4.7274\text{CO} + 4.3016\text{CO}_2 + 1.7109\text{CH}_4 + 6.9712\text{H}_2\text{O} \]

\[ \text{bio} \rightarrow 6.2792\text{tar1} \]

\[ \text{bio} \rightarrow 40.8361\text{FC1} \]

• Tar cracking (Details in following slides)

• Water gas shift (Fast kinetics Biba 1978 [8])

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

• Char gasification (Hobbs 1992 [9])

  \[ \text{C} + \text{CO}_2 \rightarrow 2\text{CO} \]
  \[ \text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 \]
Tar cracking reaction

$\text{Tar}_1 \rightarrow \text{light gases} + \text{inert tar}$

<table>
<thead>
<tr>
<th>Component mass fraction</th>
<th>Seebauer 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light gases</td>
<td>0.78</td>
</tr>
<tr>
<td>$\text{Tar}_{\text{inert}}$</td>
<td>0.22</td>
</tr>
</tbody>
</table>

$\text{Tar}_1 \rightarrow 1.5709\text{CO} + 0.197\text{CO}_2 + 0.4304\text{CH}_4 + 0.6704\text{H}_2 + 0.22\text{Tari}$

- Both $\text{tar}_1$ and $\text{tari}$ are considered to be benzene
- The global reaction is developed for biomass pyrolysis in inert environment (N2) at moderate temperatures
Comparison with NREL experiments, 1023K Steam blown bed

CO concentration

CO2 concentration

Ctari concentration
Comparison with NREL experiments, 1023K
Steam blown bed

The tar cracking mechanism of Seebauer 1999 over-predicts the produced inert tars by two orders of magnitude
Levoglucosan identified as the major tar species present after devolatilization [10]

Global tar cracking mechanism in a steam environment, based on levoglucosan cracking

Benzene assumed as the major inert tar species

Tar cracking mechanism was modified using a reactor network model employing the Ranzi mechanism to represent the LVG decomposition pattern in the absence of oxygen

\[
\text{Tar1(LVG)} \rightarrow 3.27\text{CO} + 0.2\text{CO}_2 + 0.65\text{CH}_4 + 1.1\text{H}_2 + 2.68\text{H}_2\text{O} + 0.01038\text{Tar1(Benzene)}
\]
Comparison with NREL experiments, 1023K

Steam blown bed
Comparison with NREL experiments, 1023K Steam blown bed

- Tar production is predicted accurately
- Discrepancies for CO2, H2 and H2O
Reacting vs non-reacting hydrodynamics
Summary and future work

- Ongoing work towards validation of a reacting CFD methodology for biomass gasification in a steam environment

- Use of tools employing detailed chemistry to extract information about the global chemical mechanisms implemented in CFD

- Revisit the devolatilization mechanism by implementing more detailed schemes

- Potential effect of the emulsion phase on the water gas shift reaction

- Enhancement of reactor network models employing detailed chemistry by feeding back information about gas-solids mixing obtained from CFD
References


