Modelling of Biomass Pyrolysis

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Biomass Conversion Processes

Biomass

Thermo-chemical conversion
- Combustion (in presence of excess air) → Heat energy
- Gasification (in presence of partial air and steam) → Syngas and Fuel gas
- Pyrolysis (in inert atmosphere) → Bio-oil, Bio-char and Fuel gas
- Hydrothermal liquefaction (in presence of high pressure water) → Bio-oil

Bio-chemical conversion
- Hydrolysis-Fermentation → Bioethanol
- Anaerobic digestion → Biogas
Pyrolysis Process Technologies

![Pyrolysis Process Technologies Diagram](image-url)
Multi-Scale Modelling

- Kinetic Model
- Particle Model
- Cold Flow Model
- Reactor Model

Diagram showing the relationships between Biomass, Primary Tar (T1), Secondary Tar (T2), Gas, and Char.
Particle Model

- **Particle Size**
  - Temp. = 834°C
  - 2 mm, 4 mm, 6 mm

- **Temperature**
  - Particle dia. = 4 mm
  - Model (T=459 OC), Model (T=627 OC), Model (T=732 OC)

- **Moisture Content**
  - Dry biomass density (kg/m³)
  - 0%, 10%, 20%

- **Shrinkage**
  - Biomass mass fraction
  - With shrinkage, Without shrinkage
Granular Flow Modelling

Continuity:
\[
\frac{\partial (\alpha_q \rho_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \bar{v}_q) = 0
\]

Gas momentum:
\[
\frac{\partial (\alpha_s \rho_s \bar{v}_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s \bar{v}_s \bar{v}_s) = -\alpha_s \nabla p + \nabla \cdot \bar{\tau}_s + \alpha_s \rho_s \bar{g} \rho + \sum_{i=1}^{N} R_{gs}
\]

Solid momentum:
\[
\frac{\partial (\alpha_s \rho_s \theta_s \bar{v}_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s \theta_s \bar{v}_s \bar{v}_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \cdot \bar{\tau}_s + \alpha_s \rho_s \bar{g} \rho + \sum_{i=1}^{N} R_{ls}
\]

Solid granular temp.:
\[
\frac{3}{2} \frac{\partial (\alpha_s \rho_s \theta_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s \theta_s \bar{v}_s) = -(p_s I + \bar{f}_s) : \nabla \bar{v}_s + \nabla \cdot (\kappa_s \nabla \theta_s) - \gamma_{s} + \Phi_{ls}
\]
Circulating Fluidized Bed (CFB)
Gas-Solid Flow in Riser

Radial profile

Axial profile
Effect of Boundary Condition

Inlet in experiments

Inlet configuration in 2D CFD model

Radial profile predicted by 2D CFD model (Benyahia et al., 2000)
Effect of Boundary Condition

Inlet config.-1 (BC-A)

Inlet config.-2 (BC-B)

Inlet config.-3 (BC-C)
Effect of Boundary Condition

Inlet config.-1 (BC-A)  
Inlet config.-2 (BC-B)  
Inlet config.-3 (BC-C)

Graphs showing mean solid velocity and mean solid volume fraction across different radial positions for each boundary condition.
Effect of Boundary Condition

Inlet config.-1 (BC-A)  Inlet config.-2 (BC-B)  Inlet config.-3 (BC-C)

Neither of these BCs represents true experimental kinetic energy of phases at inlet
So where is the challenge?
Need for Multiscale Drag Model

Formation of Clusters

Fluid flows around the clusters without penetration

How to model the effect of clusters

Wen-Yu and Ergun drag models: Do not capture effect of clusters

Significant Drag Reduction
Gidaspow’s Drag Model

The figure illustrates the behavior of solid particles in a riser, with graphs showing the mean solid volume fraction and mean solid velocity as functions of the radial position. The simulations are compared with experimental data, highlighting the accuracy of 3D and 2D models.
Derivation of Multiscale Drag Models: Available Approaches

**SGS**
- Fine grid periodic simulations
- Derive closure models for coarse grid simulations

**EMMS**
- Gas-solid interactions calculated by local flow conditions + empirical cluster diameter correlations

**DNS**
- Gas-particle interactions are resolved at surface of particles
EMMS Framework

Three pseudo phases

Individual particles in dilute gas phase

Particles in dense cluster phase

clusters as a large particle in gas phase

\[ \beta_{EMMS} = \frac{\varepsilon^2}{U_s} F_D = \frac{\varepsilon^2}{U_s} (m_c F_c + m_f F_f + m_i F_i) \]

c = cluster; f = dilute phase; and i = dense phase; \( \varepsilon \) = voidage; \( U_s \) = superficial slip velocity; \( m_c, m_f \) and \( m_i \) = number of particles per unit volume in cluster, dilute and dense phases; \( F_c, F_f \) and \( F_i \) = force per unit volume in cluster, dilute and dense phases
EMMS Framework: Drag Forces

\[ m_c F_c = \left[ \frac{f(1-\varepsilon_c)}{\pi d_p^3} \right] \left[ C_{Dc} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sc}^2 \right] \]

\[ m_f F_f = \left[ \frac{(1-f)(1-\varepsilon_f)}{\pi d_p^3} \right] \left[ C_{Df} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sf}^2 \right] \]

\[ m_i F_i = \left[ \frac{f}{\pi d_{cl}^3} \right] \left[ C_{Di} \frac{\pi}{4} d_{cl}^2 \frac{\rho_f}{2} U_{si}^2 \right] \]

\[ C_{D,Wen-Yu} = C_{D0} \varepsilon^{-4.7} \quad \text{and} \quad C_{D0} = \frac{24}{Re_p} (1 + 0.15 Re_p p^{0.687}) \]

\( \varepsilon_c = \text{voidage in dense phase}; \ \varepsilon_f = \text{voidage in dilute phase}; \ f = \text{cluster fraction or fraction of volume occupied by clusters}; \ d_{cl} = \text{cluster diameter}; \ U_{sc}, U_{sf} = \text{superficial slip velocities in dense and dilute phase}; \ U_{si} = \text{slip velocity between dilute phase and dense cluster} \)
EMMS and Gidaspow Model

<table>
<thead>
<tr>
<th></th>
<th>Low solid flux</th>
<th>High solid flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle dia. ($d_p$)</td>
<td>54 µm</td>
<td>76 µm</td>
</tr>
<tr>
<td>Density</td>
<td>930 kg/m³</td>
<td>1712 kg/m³</td>
</tr>
<tr>
<td>Solid mass flux ($G_s$)</td>
<td>14.3 kg/m²s</td>
<td>489 kg/m²s</td>
</tr>
<tr>
<td>Superficial gas velocity ($U_g$)</td>
<td>1.52 m/s</td>
<td>5.2 m/s</td>
</tr>
</tbody>
</table>
Verification of EMMS: Lattice Boltzmann

Particles forming a random configuration

Particles forming a cluster
- Known cluster size, cluster fraction and solid volume fractions

Graphs showing normalized drag against overall voidage and particle Reynolds number.
CFD Predictions at Low Solids Flux
CFD Predictions at High Solids Flux
## CFD Model Parameter

<table>
<thead>
<tr>
<th>Properties</th>
<th>Cellulose</th>
<th>Sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1500</td>
<td>2560</td>
</tr>
<tr>
<td>Particle Diameter (μm)</td>
<td>250-900</td>
<td>440</td>
</tr>
<tr>
<td>Restitution coefficient</td>
<td>0.97</td>
<td>0.97</td>
</tr>
<tr>
<td>Angle of internal friction</td>
<td>35</td>
<td></td>
</tr>
<tr>
<td>Cellulose to Sand Ratio</td>
<td>0.1-1.0</td>
<td></td>
</tr>
<tr>
<td>$U_{mf}$ (sand) (m/s)</td>
<td>0.145</td>
<td></td>
</tr>
<tr>
<td>$U_i/U_{mf}$</td>
<td>1-3</td>
<td></td>
</tr>
</tbody>
</table>

![Diagram of the air inlet and outlet with dimensions](image-url)
Sample Results

a) Cellulose

b) Sand
Volume Fraction Profiles

a) Air

b) Cellulose

c) Sand
Segregation of Sand and Biomass
Model Predictions

(a) Product Yield (wt. %) vs. Reactor Temperature (°C) with $u = 0.73$ m/s, Dia. = 0.4 mm

(b) Product Yield (wt. %) vs. Superficial gas velocity ($u_g$) at $T = 500°C$, Dia. = 0.4 mm

(c) Product Yield (wt. %) vs. Biomass particle diameter (mm) at $T = 500°C$, $u = 0.63$ m/s
Pyrolysis Process Model
Kinetics of Pyrolysis Process

- Experimental TGA data at heating rates between 5 to 250 K/min has been obtained for three different particle sizes (<45, 75 to 106 and 300 to 425 μm)
- Imaging intermediate and final solid residues formed during pyrolysis to get an insight into volatilization process
- Formation of open pore structure under different heating rates affects the values of frequency factor and its dependence on temperature
Kinetics of Pyrolysis Process

- Biomass is a heterogeneous solid material and its pyrolysis is modelled using distributed activation energy model (DAEM).

\[ \alpha = \sum_{i=1}^{3} c_i \left( 1 - \int_0^{\infty} \exp \left[ - \int_{T_0}^{T} \frac{A_0}{\beta} T^m \exp \left( - \frac{E}{RT} \right) dT \right] dE \right) \]

- Here, ‘\( \alpha \)’ is the fraction of volatiles released and is modelled as a linear combination of volatilization of three pseudo components having weight fraction \( C_i \).

- The values of \( m \) and \( C_i \) have been adjusted to fit the volatilization profile of pine. The activation energies have not been adjusted.

![Experimental and modelled data](image1)

![Predicted volatilization profile](image2)
Pyrolysis Process

1: K-Tron Gravimetric feeder
2: Gas pre-heater
3: Screw Feeder
4: Fluidized Bed reactor
5: Cyclones
6: Char collection Vessel
7: Fixed Bed reactor followed by three heat exchangers