Computational fluid dynamics simulations of biomass fast pyrolysis in a gas-solid vortex reactor


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Outline

• Biomass fast pyrolysis
• Gas-Solid Vortex Reactors (GSVR)
• Reactive GSVR Design
• Cold flow experiments & simulations
  – Pie vs Full geometry comparisons
• Reactive Simulations
  – Reaction mechanism & simulation details
  – Product yields
  – Radial segregation
• Conclusions & future work
Short gas residence time
Effective heat transfer between gas and solid
Fast removal of generated bio-oil vapours & rapid condensation
Gas-Solid Vortex Reactors

Rotating Fluidized Beds In Static Geometry

Centrifugal Drag

Gas-Solid slip velocities

Packed beds

Process intensification in terms of heat & mass transfer

Short Gas Residence time
Proof of concept, first reactive GSVR

Diagram:
- $L_c = 1\ mm$
- $\gamma = 10^\circ$
- $D_g = 30\ mm$

Dimensions:
- $D_f = 20\ mm$
- $L_R = 15\ mm$
- $D_j = 125\ mm$
- $A - B$
- $A - B$

Image of a fabricated reactive GSVR component.
Reduced backflow due to profiled bottom plate

Pressure drops
~ 9 kPa (slots)
~ 20 kPa (total)

Uniform velocities across slots
Solid: 0.5 mm diameter Aluminium particles

Gas: Compressed Air

Stable, packed, rotating bed of ~ 7mm height
Simulation Geometries

Full Geometry

~ 2.5 x 10^6 cells

Pie Geometry

~ 0.25 x 10^6 cells
### Simulation Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Full Geometry</th>
<th>Pie Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air inlet Temp (K)</td>
<td>289</td>
<td></td>
</tr>
<tr>
<td>Air inlet flow (kg s(^{-1}))</td>
<td>0.0143</td>
<td>0.00179</td>
</tr>
<tr>
<td>Aluminium loading (kg)</td>
<td>0.0107</td>
<td></td>
</tr>
<tr>
<td>Aluminium density (kg m(^{-3}))</td>
<td>2700</td>
<td></td>
</tr>
<tr>
<td>Aluminium dp (m)</td>
<td>0.0005</td>
<td></td>
</tr>
<tr>
<td>Aluminium feeding</td>
<td>Via UDF (0.0385 &lt; r &lt; 0.0395 m)</td>
<td></td>
</tr>
<tr>
<td>Turbulence Model</td>
<td>Re-Normalization Group k-(\epsilon) (KE-RNG)</td>
<td></td>
</tr>
<tr>
<td>Time Step (s)</td>
<td>2 X 10(^{-5})</td>
<td>10(^{-4})</td>
</tr>
</tbody>
</table>

**Simulation Procedure (using ANSYS FLUENT v15.0.7):**

Gas only simulation $\rightarrow$ Solid feeding in developed gas field via UDF $\rightarrow$ stable bed data
Pie-geometry can be chosen for computational ease.
### Reactive CFD Simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen inlet Temp (K)</td>
<td>842</td>
</tr>
<tr>
<td>Nitrogen inlet flow (kg hr(^{-1}))</td>
<td>18</td>
</tr>
<tr>
<td>Biomass Loading (kg)</td>
<td>0.001 (batch feed)</td>
</tr>
<tr>
<td>Biomass feed temp (K)</td>
<td>842</td>
</tr>
<tr>
<td>Time Step (s)</td>
<td>(10^{-4})</td>
</tr>
<tr>
<td>Turbulence Model</td>
<td>k-ε RNG</td>
</tr>
<tr>
<td>Primary Phase</td>
<td>Gas Mixture (N(_2), pyrolysis gas, bio-oil vapours)</td>
</tr>
<tr>
<td>Secondary Phase – I (Granular)</td>
<td>Biomass Phase</td>
</tr>
<tr>
<td>Secondary Phase – II (Granular)</td>
<td>Char Phase</td>
</tr>
<tr>
<td>Interphase interactions</td>
<td>Various closure models in FLUENT Drag: Gidaspow correlation Heat Transfer: Gunn Correlation</td>
</tr>
</tbody>
</table>
Fast Pyrolysis Reaction Mechanism

Biomass (dry) → v.Hemicellulose → a.Hemicellulose
(47 %)

v.Cellulose → a.Cellulose
(36 %)

v.Lignin → a.Lignin
(17 %)

Biomass Phase
dp = 0.5 mm

Char Phase
dp = 0.2 (0.3 mm)

Char_c + Gas

Char_h + Gas

Char_l + Gas

Bio-oil → Gas

Bio-oil → Gas

Bio-oil → Gas

### Key Results

(Results scaled for the full reactor configuration)

<table>
<thead>
<tr>
<th>Product Distribution</th>
<th>Previous (2-D) Simulations$^1$</th>
<th>Current Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>Char</td>
<td>14 – 17 %</td>
<td>20.92 %</td>
</tr>
<tr>
<td>Bio-oil</td>
<td>73 – 76 %</td>
<td>68.19 %</td>
</tr>
<tr>
<td>Pyrolysis Gas</td>
<td>8.5 - 9.5 %</td>
<td>10.89 %</td>
</tr>
</tbody>
</table>

Radial Segregation

- Density ratio: 0.9 & dp ratio: 2.5 show positive radial segregation

- Streamlines near the outlet indicate likeliness of char exiting the reactor as compared to biomass

- Segregation is transient and char bed moves radially outwards as biomass reacts.

- To sustain segregation and reduce char residence time in reactor, continuous biomass feeding could be implemented.

Solids v.f. profiles displayed at axial plane: z = 0.01 m

Biomass
dp = 0.5 mm
\( \rho = 450 \text{ kg m}^{-3} \)

Char
dp = 0.2 mm
\( \rho = 500 \text{ kg m}^{-3} \)
Radial Segregation – II

Biomass
$dp = 0.5 \text{ mm}$
$\rho = 450 \text{ kg m}^{-3}$

Biomass
$dp = 0.3 \text{ mm}$
$\rho = 500 \text{ kg m}^{-3}$

Solids v.f. profiles displayed at axial plane: $z = 0.01 \text{ m}$
Conclusions & Future Work

• Pie-geometry suitable for running qualitative reactive simulations. Detailed experimental comparison with simulations necessary.

• Simulations indicate transient radial char and biomass segregations within a range of biomass to char diameter ratios. Leads to process intensification favorable for fast pyrolysis.

• Char, bio-oil yields lesser than those in previous (2-D) reactive simulations, indicating strong influence of end-wall effects.

• Comprehensive reaction mechanisms coupled with CFD for studying favourable products formation.
Acknowledgements

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Research Foundation Flanders
Opening new horizons

Vlaams Supercomputer Centrum
Backup Slides
Reactive GSVR Unit
<table>
<thead>
<tr>
<th>Reaction$^a,b$</th>
<th>$\Delta H_{\text{rxn}}$ (kJ/kg)</th>
<th>$A_f$ (1/s)</th>
<th>$E_A$ (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL$_v$ → CL$_a$</td>
<td>0</td>
<td>$2.80 \times 10^{19}$</td>
<td>242.4</td>
</tr>
<tr>
<td>HC$_v$ → HC$_a$</td>
<td>0</td>
<td>$2.10 \times 10^{16}$</td>
<td>186.7</td>
</tr>
<tr>
<td>LG$_v$ → LG$_a$</td>
<td>0</td>
<td>$9.60 \times 10^{8}$</td>
<td>107.6</td>
</tr>
<tr>
<td>CL$_a$ → Tar</td>
<td>255</td>
<td>$3.28 \times 10^{14}$</td>
<td>196.5</td>
</tr>
<tr>
<td>HC$_a$ → Tar</td>
<td>255</td>
<td>$8.75 \times 10^{15}$</td>
<td>202.4</td>
</tr>
<tr>
<td>LG$_a$ → Tar</td>
<td>255</td>
<td>$1.50 \times 10^{9}$</td>
<td>143.8</td>
</tr>
<tr>
<td>CL$_a$ → 0.35 Char$_c$ + 2.6 Pgas</td>
<td>−20</td>
<td>$1.30 \times 10^{10}$</td>
<td>150.5</td>
</tr>
<tr>
<td>HC$_a$ → 0.6 Char$_h$ + 1.6 Pgas</td>
<td>−20</td>
<td>$2.60 \times 10^{11}$</td>
<td>145.7</td>
</tr>
<tr>
<td>LG$_a$ → 0.75 Char$_l$ + Pgas</td>
<td>−20</td>
<td>$7.70 \times 10^{6}$</td>
<td>111.4</td>
</tr>
<tr>
<td>Tar → 4Pgas</td>
<td>−42</td>
<td>$4.25 \times 10^{6}$</td>
<td>108.0</td>
</tr>
</tbody>
</table>
Biomass Experiments - I

Nitrogen:
- 12 – 29 g/s
- Slot vel = 75 – 140 m/s

Pinewood
- 500 kg/m³
- Max dimension: 1.5 mm
- 8-10 gm biomass

- Start gas flow rate
- Feed biomass particles
- Wait till bed stabilizes and no particles entrain with gas
- Record PIV data
- 3 repeats
Results - II

Full geometry simulations closer to the experimental data; both numerically and the trend as well.
Velocities in the bed and freeboard match excellently. Near exhaust, values differ, probably due to effect of outlet size (r=0.01m) & shape.

Slightly expanded bed observed in pie geometry: non-inclusion of adjacent slot effects which is more pronounced in full geometry.