Computational study on biomass fast pyrolysis: Hydrodynamic effects on the performance of a laboratory-scale fluidized bed reactor

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Background and Motivation (1)

Thermochemical conversion of biomass based on fast pyrolysis

- High yield and composition of raw oil are key, so commercial risk and economics depend on accurate performance predictions.
- Most available basic lab data are from bubbling fluidized bed reactors (FBRs).
- Good physics-based models are necessary for interpreting, scaling up lab experiments.
Background and Motivation (2)

How should lab FBR data be interpreted/analyzed?

FB Hydrodynamics directly impact:

1. Particle residence time
2. Gas residence time
3. Particle heating rate
4. Particle attrition/fragmentation
5. Particle and ash elutriation
6. Particle segregation

All the above significantly impact raw oil yield and composition.

Note: Bubble boundary depicted where void fraction > 0.65

Approach (1): MFIx simulations of FBR pyrolysis

Pyrolysis reactor physics

Two-Fluid CFD Model

- Eulerian-Eulerian
- Kinetic theory of granular flow
- 3D cylindrical mesh
- DLSODA ODEPACK chemistry solver
  - First order irreversible Arrhenius rates
  - Liden 1988 biomass pyrolysis kinetics

\[
\text{wood} \xrightarrow{k1} \text{Tar} \xrightarrow{k3} \text{gas} \quad \text{gas} \xrightarrow{k2} \text{gas + char}
\]
Use simplified reactor models to ‘compress’ essential hydrodynamic information from MFIX and combine it with pyrolysis chemistry

- Quantify impact of bubbles and bed solids circulation on biomass solids and py vapor RTDs
- Identify major reaction/mixing zones needed to understand/approximate performance trends
- Relate solids and gas RTDs to predict trends for how biomass particle properties and reaction chemistry impact overall yields
- Utilize low-order models for rapid studies of operating/design parameter sweeps
Approach (3): Compare MFIIX predictions for lab-scale FB pyrolysis reactor with literature and experiments

- Target: Select NREL lab-scale pyrolysis experiment as typical lab-scale example
- Key steps:
  - Simulate expected particle and gas RTDs with MFIIX including segregation and elutriation
  - Are MFIIX mixing patterns consistent with the literature?
  - Can existing FB correlations capture MFIIX predicted RTD trends?
  - When chemistry is added, do predicted bio-oil yields agree with experiments?
  - Are MFIIX improvements needed?


Approach (4): NREL lab pyrolyzer details

- Target: Fluidized bed particle studies used to verify model
- Key steps:
  - Reproduce exp. particle residence time distribution (RTDs)
  - Relate impact of char elutriation and mixing on RTDs
  - Reproduce impact of solids segregation on mixing

<table>
<thead>
<tr>
<th>Property</th>
<th>Units</th>
<th>Mixing Study Park &amp; Choi 2013</th>
<th>RTD Study Berruti 1988</th>
<th>NREL Exper.</th>
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</thead>
<tbody>
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<td>Particle diameter (Sand)</td>
<td>m</td>
<td>$387 \times 10^{-6}$</td>
<td>$710 \times 10^{-6}$</td>
<td>$500 \times 10^{-6}$</td>
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<td>Fluidizing $\mathrm{N}_2$ (range)</td>
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<td>Minimum fluidization</td>
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<td>Angle of repose</td>
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<td>Friction coefficient</td>
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<td>0.1</td>
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</tbody>
</table>


Preliminary MFIX Results(1): Biomass Particle RTD

Axial slice of 3D bubbling bed simulation
Residence time distribution (RTD) study

Comparison of simulation and experiment
RTD (Berruti 1988)
Bubbles are the main mixing mechanism

More bubbles, more char/sand mixing

Char layer decreases with gas flow

Simulated tracers track char/gas mixing and RTD's

Comparison of simulation and experiment char mixing (Park and Choi 2013)
Preliminary MFIX Results (3): Biomass Particle Elutriation

Particle size and density must be selected carefully such that elutriation will occur.

Biomass particle size

Biomass particle density
As inlet gas flow increases, biomass particle RTD converges to a limit.

RTD whole reactor, biomass particles

CDF normalized F-curve $[C(t)]$

0 0.2 0.4 0.6 0.8 1

0 5 10 15 20 25 30

time (sec)

2umf
3umf
4umf
5umf
6umf
7umf
Preliminary MFiX Results (5): Yield Convergence with Chemistry

Liden lumped kinetics in MFiX reactor and low order reactor model predict tar experiment yields

![Graph showing yield vs. time for various products](image-url)

- **Product**: tar, gas, char, wood
- **Low order**: tar, gas, char, wood

**Yield**: \( \frac{C}{C_0} \)

**Time**: (s)

**Yield (C/C₀)**

0 0.2 0.4 0.6 0.8 1.0 1.2 1.4

0 2 4 6 8 10 12 14 16 18

**Time (s)**
Preliminary Low-Order Results: Chemistry + MFiX Hydrodynamics (Possible ‘Hybrid’ Modeling Approach)

1. Use MFiX gas and biomass RTDs to create zone reactor model approximation

2. Use zone model + Liden kinetics to predict yields

How do the models compare with experimental data?

![Bar chart showing comparison between experimental data and different models (MFiX, Low Order, Hybrid) for tar, gas, char, and wood production.](image-url)
Concluding remarks

- Quantifying the combined effects of hydrodynamics and chemistry is essential in utilizing lab-scale biomass pyrolysis reactor data for scale up.
- Biomass particle properties and fluidization intensity have major impacts on product yields.
- A key question remains: Is there a single combination of biomass feed particle size and fluidization intensity where tar yield is maximized?
- Two-fluid codes like MFIIX can yield useful details about pyrolyzer hydrodynamics and gas and solid RTDs but improvements to the physics are still needed.
- Combining MFIIX hydrodynamics with low-order chemistry models appears to offer potential benefits.
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Questions?

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