Particle-scale modeling of heat transfer in a double screw pyrolyzer

Fenglei Qi and Mark Mba Wright*

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* Presenting author: markmw@iastate.edu
Fast pyrolysis reactors

- Fluidized bed reactors are commonly used
  - High heat transfer rate
  - Relatively mature design experience
  - Simple geometry
  - Capability for scale-up
  - Ease of operation
  - High bio-oil yield

Drawback: Large amount of hot inertial fluidized gas is needed

Bubbling fluidized bed
He et al. (2016)

Double screw reactor
Brown and Brown (2012)

Horizontal stirred bed reactor
Lago et al. (2015)

Vertical stirred bed reactor
Xi et al. (2015)
Empirical knowledge: Double screws generate better mixing between particles
- Adding heat carrier particles to enhance biomass particle heating rates
- Flexible mass feeding ratio of biomass to heat carrier
- Comparable performance to the fluidized bed reactors in terms of bio-oil yield at low feeding rate ($fb = 1.0 \text{ kg/h}$) reported by Brown and Brown (2012)
Fundamental understanding of granular flow and heat transfer physics in the reactor

- Experimental work by Kingston and Heindel (2014a, 2014b)

- Cold flow
- Limited tracking number of particles (X-ray)
- High cost of time and equipment

Our goal: Developing an Discrete Element Method (DEM) to resolve particle-scale physics to gain better insight of granular flow and heat transfer physics
Discrete element method (DEM)

- DEM considers each particle as an entity in a collection of particles and resolves each particle motion based on Newton’s equations of motion.

Translational

\[
m_i \frac{dv_i}{dt} = \sum_j F_{ij}^c + \sum_k F_{ik}^{nc} + F_i^f + F_i^g
\]

Rotational

\[
I_i \frac{d\omega_i}{dt} = \sum_j (T_{t,ij} + T_{r,ij})
\]
Simulation carried out by LIGGGHTS

- Particle residence time distribution (RTD) and mixing degree (M) along the axial direction were investigated.

Particle-scale heat transfer mechanisms

- Lumped capacity model

\[
m_i c_{p,i} \frac{dT_i}{dt} = \sum_j Q_{ij} + Q_{f,c} + Q_{f,r}
\]

- Particle-particle conduction
- Particle-fluid-particle conduction
- Particle-particle radiation
- Particle-fluid convection (forced or natural)
- Particle-fluid radiation

The contribution of each heat transfer pathway depends on the particulate flow parameters such as void fraction, particle thermal properties and gas interactions.
Particle-scale heat transfer model

- Particle-particle conduction by Zhou et al. (2004)

\[ Q_{ij}^{pp} = \frac{4\pi r_c c (T_j - T_i)}{k_{p,i} + k_{p,j}} \]

\[ c = \left( \frac{E_{ij}}{E_{ij,0}} \right)^{1/5} \]

- Particle-fluid-particle conduction by Cheng et al. (1999)

\[ Q_{ij}^{pfp} = (T_j - T_i) \int_{r_{stij}}^{r_{sfj}} \frac{2\pi rdr}{\left( \sqrt{R^2 - r^2} - r(R + H)/r_{ij} \right) \cdot (1/k_{pi} + 1/k_{pj}) + 2[(R + H) - \sqrt{(R^2 - r^2)}/k_f} \]

- Particle-particle radiation by Cheng and Yu (2013)

\[ Q_{ij}^{rad} = \sigma \frac{(T_j^4 - T_i^4)}{1 - \epsilon_{r,i} A_i + \frac{1}{A_i F_{ij} + [1/(A_i F_{iR}) + 1/(A_j F_{jR})]^{-1}} + \frac{1 - \epsilon_{r,j}}{\epsilon_{r,j} A_j}} \]

\[ F_{ij} + F_{iR} = 1 \]

\[ F_{ij} = F_{ji} \]
Interactions between spherical particle and wall

- Triangle meshes are employed to render surfaces of reactors

- Soft sphere model is applied to resolve the collision between particles and triangle meshes
Sphere-triangle mesh heat transfer

- Effective circular surface of triangle mesh

- Single cone boundary model
Model validation: Heat transfer in pack beds

- Effective thermal conductivity is independent of cell size when $x_i > 8d_p$

- Effective thermal conductivity (ETC) is calculated as

$$k_e = \frac{q}{(T_h - T_c) / H}$$

- ETC is given by

$$k_p = 0.83 \text{ W/m·K}, \quad k_f = 0.028 \text{ W/m·K}$$

- Parameters:

$$\varepsilon_p = 0.56, \quad d_p = 2 \text{ mm}$$
A good agreement is observed between model predictions and experimental measurements.
Thermal properties

<table>
<thead>
<tr>
<th>Material</th>
<th>Red Oak</th>
<th>Sand</th>
<th>Steel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Temperature $T_0$ (K)</td>
<td>300</td>
<td>844</td>
<td>788</td>
</tr>
<tr>
<td>Conductivity ($\frac{W}{m\cdot K}$)</td>
<td>0.2</td>
<td>1.3</td>
<td>38</td>
</tr>
<tr>
<td>Specific heat capacity ($\frac{W}{kg\cdot K}$)</td>
<td>2023</td>
<td>730</td>
<td>490</td>
</tr>
<tr>
<td>Emissivity</td>
<td>0.9</td>
<td>0.8</td>
<td>0.8</td>
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</tbody>
</table>

Operation conditions: Counter rotating pumping down, $\omega=40$ rpm, $P/D=1.25$, $d_p = 2$ mm
Distributions of particle and temperature in axial directions at different feed rates

- Temperature distribution aligns with particle distribution at high feeding rates
- Particle mixing has limited effects on heat transfer at low feed rates

High feed rate $f_b=3.5$ kg/h

Low feed rate $f_b=1.0$ kg/h
Distributions of particle and temperature in axial directions with different particle sizes

- Similar particle & temperature distributions are observed with different particle sizes
Distributions of particle and temperature in axial directions with different rotation speeds

- In pitch 7, more uniform temperature is achieved at smaller rotation speed due to increased residence time
In current reactor design and operation conditions, it is predicted only one case ($d_p=1.0$ mm, $f_b=1.0$ kg/h) achieves steady temperature before the reactor outlet.
The range of biomass particle heating rate in the reactor is between 20 and 50 K/s in current operation conditions.

Increasing rotation speed improves biomass heating rate, while increasing biomass feed rate decreases the heating rate.

Biomass heating rate is not affected by biomass particle size in the range of 1-2 mm.
Summary

- A thermal DEM model considering particle-scale heat transfer was developed and validated in this research.

- Biomass heating rate was predicted within the range of 20-50 K/s in the double screw reactor at current operation conditions.

- The influences of the operating conditions on the temperature profiles in the reactors were investigated showing that higher rotation speed and longer residence time are favorable for the heat transfer at constant feed rate while decreasing feed rate could enhance the heating process of biomass particle.

- Biomass heating rate is not affected by biomass particle size in the range of 1-2 mm when feed rate is greater than 2 kg/h.
Acknowledgement

- Funding: National Science Foundation EPSCoR program

- Dr. Robert Brown, Dr. Qi Dang, Tannon Daugaard and all other colleagues in the BEI and CoMFRE at Iowa State University.


Thank you

Question?
Backup slides
Motivation: biomass fast pyrolysis modeling

Question: what physics and scales should be considered in the mathematical model development for fast pyrolysis modeling?

Motivation: biomass fast pyrolysis modeling

<table>
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<th>Scale</th>
<th>Complexity</th>
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<tr>
<td>Kinetic modeling</td>
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<tr>
<td>Single particle modeling</td>
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<tr>
<td>Particle flow modeling</td>
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</table>

- Kinetic modeling
  - Temperature, Reaction time

- Single particle modeling
  - Intra-particle heat and mass transfer
  - Internal Mass Transport

- Particle flow modeling
  - Eulerian method
  - DEM method
  - Particle-particle and particle-gas interactions
Model validation

Biomass: Blue, Heat carrier: Red

Operation conditions: Counter rotating pumping down, $\omega=40$ rpm, P/D=1.25

Experimental photo from Kingston and Heindel (2014)
Discrete element method (DEM)

- Soft sphere model (spring-dashpot model)

\[ F_{ij}^c = F_{n,ij}^c + F_{t,ij}^c \]

- Overlap in normal and tangential directions are allowed. Force-displacement models and damping models are adopted

\[ F_{n,ij}^c = -k_n \delta_n^\alpha \hat{n} + C_n (v_{rel,C} \cdot \hat{n}) \hat{n} \]

\[ F_{t,ij}^c = k_t \delta_t^\beta + C_t (v_{rel,C} \times \hat{n}) \times \hat{n} \]

\[ |F_{\text{contact},t,ij}| \leq \mu |F_{\text{contact},n,ij}| \]

Hertz-Mindlin model is employed in this research.
Particle-scale heat transfer model

- Double cones boundary model (Cheng et al., 1999)

Voronoi tessellation of a 2D packed bed
Cheng et al. (1999)

Boundary parameters are related to local void fraction in the bed

\[ r_{ij} = 0.560R \left(1 - \varepsilon_i\right)^{-\frac{1}{3}} \quad r_{sf} = \frac{R \cdot r_{ij}}{\sqrt{r_{ij}^2 + (R + H)^2}} \]
View factor

- Definition of view factor

\[ F_{ij} = \frac{1}{A_i} \int_{A_i} \int_{A_j} \frac{\cos \phi_i \cos \phi_j \, dA_i \, dA_j}{\pi L^2} \]

- Monte Carlo Method (Mont3D)

\[ F = \frac{1}{\pi w^2} \left[ \ln \left( \frac{1 + w^2}{1 + 2w^2} \right) + 4w \left( \sqrt{1 + w^2} \cdot \arctan \frac{w}{\sqrt{1 + w^2}} - \arctan w \right) \right] \]

\[ F' = 2h^2 - 2h \sqrt{h^2 - 1} - 1 \quad h = C / 2R \]
Correlations of view factor

- Very loose random packing ($\varepsilon_s = 0.56$)

\[
F_{ij} = 0.4225 \frac{d_{ij}}{R} - 0.3371
\]

\[
F_{ij} = 0.06233 \left( \frac{d_{ij}}{R} \right)^{7.051} \left( \frac{\bar{r}_{sf}}{\bar{r}_{ij}} \right)^{-7.364}
\]
Heat conduction by particle-fluid-particle is the dominant contribution to the total conductive heat transfer when \( k_p/k_f < 100 \).
Time scales

- Collision time

\[ t_{Hertz} = 2.87 \left( \frac{m^*}{v_{rel}R^*(E^*)^{2}} \right)^{1/5} \]

In order to resolve collision, computational time step is usually < 1/20 of \( t_{Hertz} \)

- Biomass residence time

\[ t_{plug\text{flow}} = \frac{L}{\omega P} \]

- Computational cost

\[ \frac{t_{plug\text{flow}}}{t_{Hertz}} \sim 10^7-10^8 \]

- Smaller Young’s modulus is used to reduce computational cost
- MPI technique is employed to simulate large particle systems
Distributions of particle and temperature in axial directions at different feeding rates

- High feeding rate ($f_b=3.5$ kg/h)
  - At high feeding rate, particle temperature distribution in transverse sections aligns with particle distribution

- Low feeding rate ($f_b=1.0$ kg/h)
  - At low feeding rate, particle mixing has limited impact on heat transfer