Modeling the Impact of BiomassParticle Size Distribution and Shape on Heating Behavior During Fast Pyrolysis

Gavin Wiggins
✉ wigginsg@ornl.gov
🌐 gavinw.me

Stuart Daw
✉ dawcs@ornl.gov

Peter Ciesielski
✉ peter.ciesielski@nrel.gov

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Problem Statement

Complex characteristics (anisotropic, non-spherical) of wood must be considered to accurately predict biomass pyrolysis.

Devolutilization of biomass particles requires sufficient heat up time to produce optimal product yields.

Microscopy of biomass feedstocks. Source: Peter Ciesielski, NREL.

SEM micrographs of real biomass particles. Source: Peter Ciesielski, NREL.
Background and Motivation

Anisotropic and heterogeneous properties of wood are often not accounted for in low-order models.

Reactor models often ignore temperature gradients within large biomass particles.
[Cui 2007, Souza-Santos 2010]

Most pyrolysis models treat wood particles as “one” size, ignoring particle size distributions from wood grinders and mills.

1-D models in literature frequently validate with experimental data for particle sizes > 6 mm, whereas typical size for fast pyrolysis in fluidized bed reactors is < 6 mm.
Accurately predict the pyrolysis of a biomass particle without using expensive HPC resources.

Use detailed 3-D microstructure models (NREL) to validate and improve low-order particle models for heat transfer in biomass particles at fast pyrolysis conditions.

Account for effects of particle size distribution and shape on heat up time of biomass particles.
Realistic 3-D particle models with microstructure

Detailed microscopy providing highly resolved species-specific microstructure.

Allows assessment of microstructure on heat/mass transfer during pyrolysis.

Enables simulations of oil yield and composition at the particle scale as functions of feedstock species, particle size distribution, and moisture.

Images courtesy of Peter Ciesielski of NREL.
Detailed particle models are computationally expensive.

- Model from XCT reconstruction
- Model with simplified microstructure
- Model with similar shape and bulk volume

Increasing computational speed
Increasing accuracy

Sphere model with similar bulk volume

Complex, 3-D particle model
Low-order particle model
Reactor-scale fast pyrolysis model

Can 1-D model replicate realistic particle heat up?

Previous work\cite{1} demonstrated importance of internal microstructure of wood particles and its affect on devolatilization.

Surface area, volume, and species specific thermal properties were key parameters in simulating realistic wood particles at fast pyrolysis conditions.\cite{1}

\begin{itemize}
  \item FEM simulation of detailed microstructural model with cell wall thermal properties
  \item FEM simulation of accurately shaped model with bulk thermal properties
  \item Low order/1-D heat transfer model appropriate shape descriptors and thermal properties
\end{itemize}

Images courtesy of Peter Ciesielski from NREL.
Approximate heat-up as 1-D conduction with bulk properties and simple boundary conditions.

\[ \rho C_p \frac{\partial T}{\partial t} = \frac{1}{r^b} \frac{\partial}{\partial r} \left( kr^b \frac{\partial T}{\partial r} \right) + g \]  

intra-particle heat conduction

Boundary condition with convection at particle surface

\[ k \frac{\partial T}{\partial r} \bigg|_{r=R} = h \left( T_\infty - T_R \right) \]

boundary condition with symmetry at particle center

\[ \frac{\partial T}{\partial r} \bigg|_{r=0} = 0 \]

Where

- \( \rho \) = density (kg/m\(^3\))
- \( C_p \) = heat capacity (J / kg·K)
- \( k \) = thermal conductivity (W / m·K)
- \( T \) = temperature (K)
- \( T_\infty \) = ambient temperature (K)
- \( T_R \) = surface temperature (K)
- \( r \) = radius (m)
- \( b \) = shape factor of 0=slab, 1=cylinder, 2=sphere
- \( g \) = heat generation (W/m\(^3\))
- \( h \) = heat transfer coefficient (W / m\(^2\)·K)
Characterizing irregular shaped particles

An equivalent diameter or characteristic length can be used to represent a measured parameter (surface area, volume, etc.) of an irregularly shaped particle.

\[
D_{SV} = \left( \frac{D_v^3}{D_s^2} \right)
\]

Sphere with same surface area to volume ratio

\[
D_S = \left( \frac{S}{\pi} \right)^{1/2}
\]

Sphere with same surface area

\[
D_L = \frac{\sqrt{S}}{\pi}
\]

Sphere with same length

\[
D_{CH} = \frac{V}{S}
\]

Characteristic volume to surface area

\[
D_V = \left( \frac{6V}{\pi} \right)^{1/3}
\]

Irregular shaped wood particle

Overall particle height

\[D_H\]
Particles classified into regimes based on Feret diameter by image analysis of 0.5 mm and 2.0 mm sieve samples.

Feret diameter ($D_F$) is the longest distance between two points on a two-dimensional plane.

More details about particle characterization provided in microstructure paper.\footnote{1}
Dsv model reproduces 3-D temperature profiles

Bulk properties from Wood Handbook used for 3-D and 1-D particle model comparison for pure heat conduction (no kinetics).

<table>
<thead>
<tr>
<th>Property</th>
<th>Loblolly Pine</th>
<th>White Oak</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>540</td>
<td>720</td>
</tr>
<tr>
<td>$k$ (W/m·K)</td>
<td>0.12</td>
<td>0.16</td>
</tr>
<tr>
<td>$h$ (W/m$^2$·K)</td>
<td>350</td>
<td>350</td>
</tr>
<tr>
<td>$C_p$ (J/kg·K)</td>
<td>$103.1 + 3.867 T$</td>
<td>$103.1 + 3.867 T$</td>
</tr>
<tr>
<td>$T_o$ (K)</td>
<td>293</td>
<td>293</td>
</tr>
<tr>
<td>$T_f$ (K)</td>
<td>773</td>
<td>773</td>
</tr>
</tbody>
</table>

Geometry for calculating equivalent diameters.

Source: [2].
Dsv model reproduces 3-D temperature profiles

Low-order Dsv model capable of reproducing surface (Ts), center (Tc), and volume average (Tv) temperature profiles of 3-D particle model.

Volume average temperature of low-order Dsv particle model matches 3-D results for a range of particle sizes.

Source: [2].
Biomass feedstock contains a range of particle sizes.

Raw data from image analysis:

- **0.5 mm sieve**
  - min = 5.3 um
  - max = 1764 um

- **2.0 mm sieve**
  - min = 3.6 um
  - max = 8085 um

Particle size distribution from image analysis:

- **0.5 mm sieve**
- **2.0 mm sieve**
Particle characterization affects temperature profile

Low-order Dsv model utilizing bulk thermal properties for loblolly pine was applied to each particle size.

Assuming biomass feedstock is same sphere size as sieve produces misleading results.

Temperature profiles from low-order model for with $D_F = 81 – 5277$ um and single sphere with $D = 0.5$ and $2$ mm.

Temperature profiles from low-order model for solid sphere.
Particle size distribution affects overall heat up time

Volume fraction of each bin used to calculate contribution to heat up time.

Accounting for entire range of particle sizes in biomass feedstock drastically affects predicted heat up time.

Similar surface area to volume ratio
Reactor models must account for size distributions.

<table>
<thead>
<tr>
<th>Products (wt. %)</th>
<th>0.5 mm sieve</th>
<th>2.0 mm sieve</th>
<th>0.5 mm sieve</th>
<th>2.0 mm sieve</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Experiment</td>
<td>Model</td>
<td>Experiment</td>
<td>Model</td>
</tr>
<tr>
<td>Total liquids</td>
<td>70.8 ± 1.1</td>
<td>72.1</td>
<td>63.5 ± 1.9</td>
<td>44.0</td>
</tr>
<tr>
<td>Char</td>
<td>9.5 ± 0.1</td>
<td>13.7</td>
<td>11.7 ± 1.3</td>
<td>8.2</td>
</tr>
<tr>
<td>Gas</td>
<td>15.5 ± 0.6</td>
<td>12.3</td>
<td>18.7 ± 0.8</td>
<td>6.5</td>
</tr>
</tbody>
</table>

Experimental data from 2-inch diameter bubbling fluidized bed reactor at NREL.

Initial model results from Dsv particle model coupled to a low-order reactor model.
Summary

- Computational models can provide information about pyrolysis conditions within small particles (very difficult in experiments)

- Sieve/mesh/screen size is not an appropriate dimension to characterize biomass particles

- Particle size and shape distributions must be accounted for to accurately predict heat up time of biomass feedstocks

- Unique shapes (aspect ratio) can be approximated as an equivalent spherical diameter

- Low-order particle model utilizing Dsv and bulk thermal properties approximates heat conduction in realistic wood particles
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Questions?

Gavin Wiggins  
✉️ wigginsg@ornl.gov  
🌐 gavinw.me

Stuart Daw  
✉️ dawcs@ornl.gov

Peter Ciesielski  
✉️ peter.ciesielski@nrel.gov


Supplemental Material
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