Modeling the Impact of Biomass Particle 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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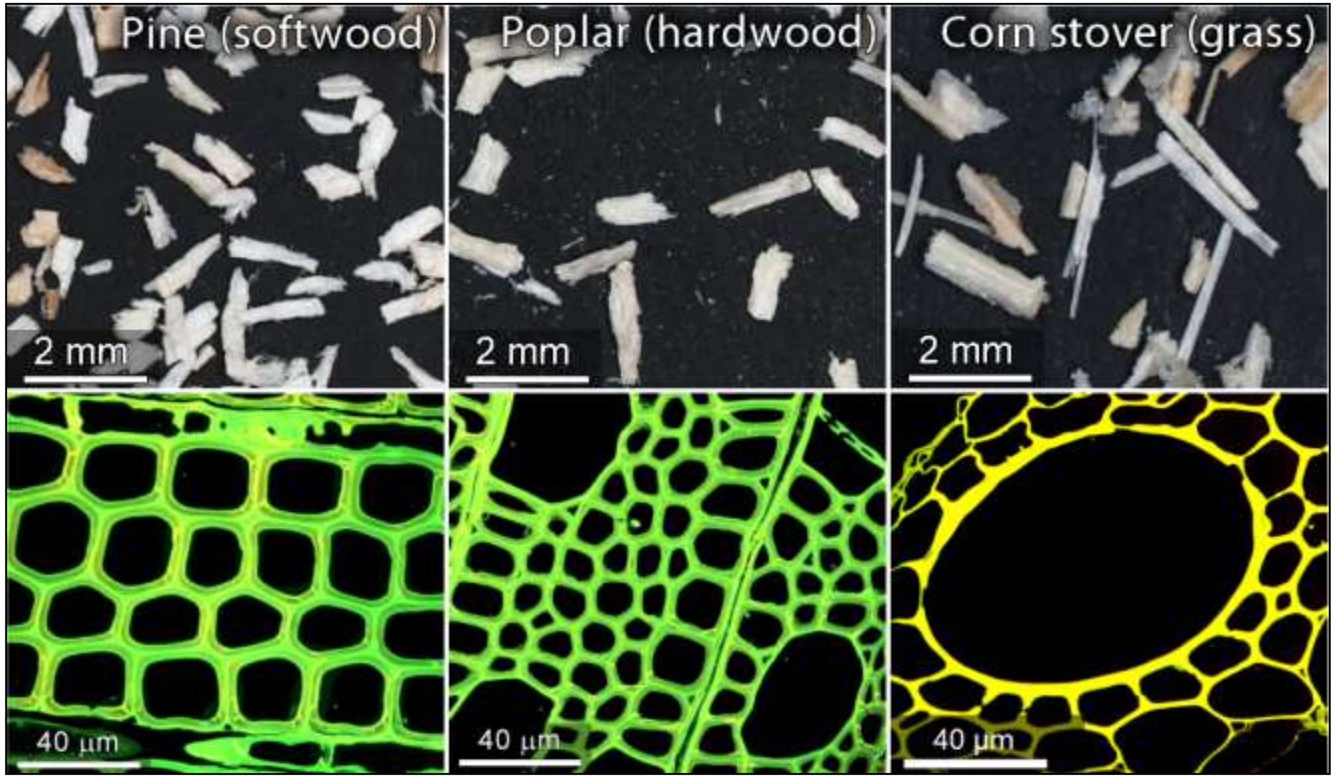
Oak Ridge National Laboratory

Computational Pyrolysis Consortium
cpcbiomass.org

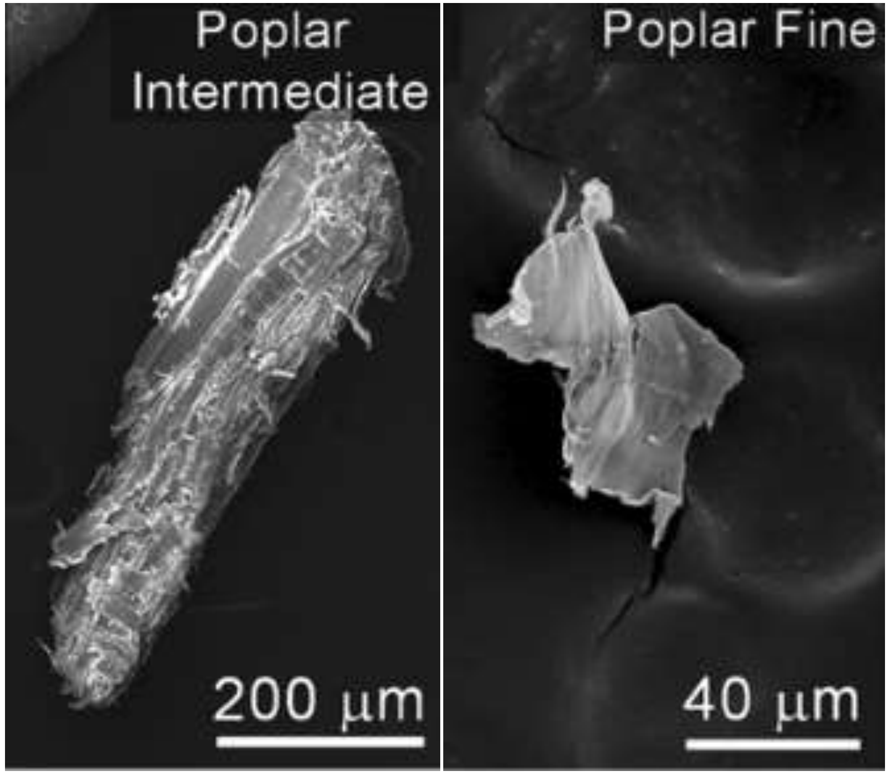
Problem Statement

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

Devolatilization 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.
[Chaurasia 2003, Babu 2004, Gronli 2000, Haseli 2011, Koufopanos 1991, Kung 1972, Larfeldt 2000, Okekunle 2011, Papadikis 2010, Prakash 2009, Pyle 1984, Sadhukhan 2009]

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.
[Di Blasi 2002, Bryden 2002, Chaurasia 2003, Cui 2007, Galgano 2003, Galgano 2004, Gronli 2000, Haseli 2011, Janse 2000, Koufopanos 1991, Kung 1972, Larfeldt 2000, Miao 2011, Papadikis 2009]

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.
[Chan 1985, Di Blasi 2003, Bridgwater 2012, Galgano 2006, Gaston 2011, Gronli 2000, Koufopanos 1991, Meier 2013, Pyle 1984, Rath 2002, Sadhukhan 2009, Trendewicz 2014]

Objectives

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.

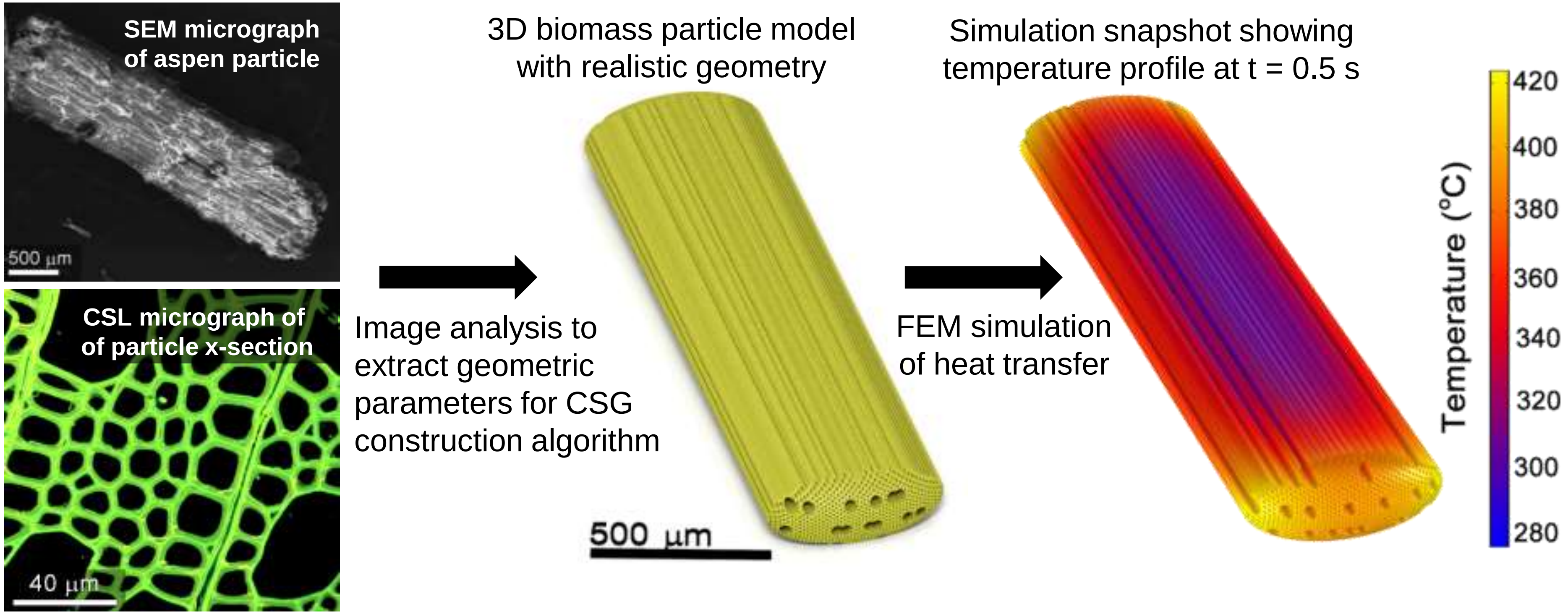
Account for effects of particle size distribution and shape on heat up time of biomass particles.

Realistic 3-D particle models with microstructure

Detailed microscopy providing highly resolved species-specific microstructure.

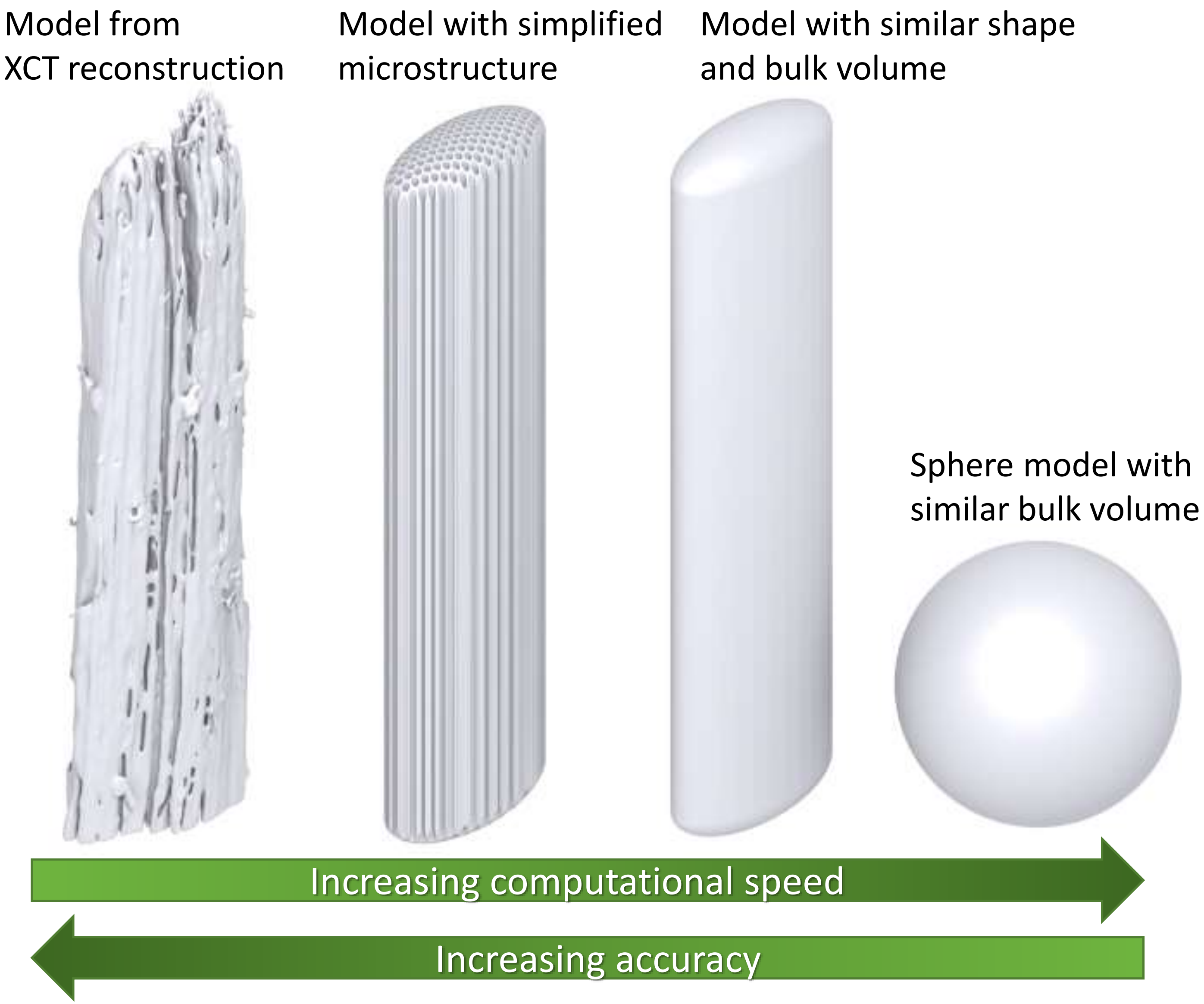
Allows assessment of microstructure on heat/mass transfer during pyrolysis.

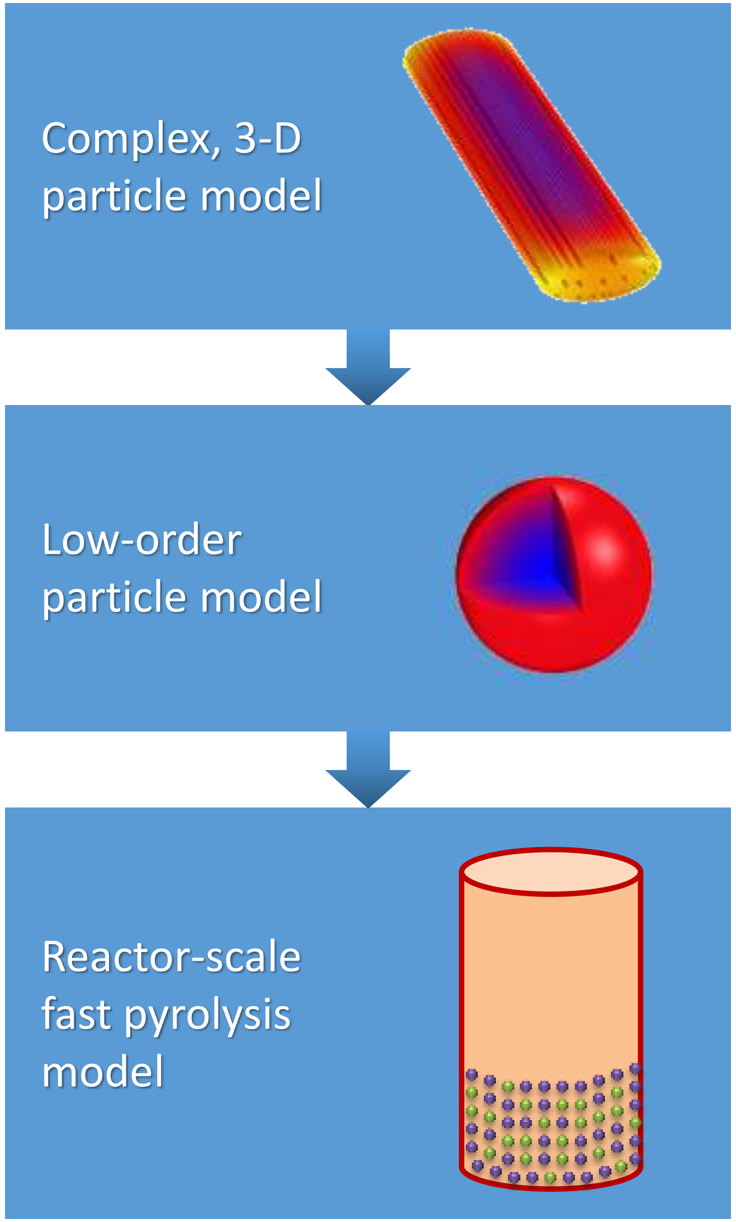
Enables simulations of oil yield and composition at the particle scale as functions of feedstock species, particle size distribution, and moisture.



Images courtesy of Peter Ciesielski of NREL.

Detailed particle models are computationally expensive





Source: Peter Ciesielski, Gavin Wiggins, Joseph Jakes, and Stuart Daw. Book chapter in "Fast Pyrolysis of Biomass" for Royal Society of Chemistry, in progress.

Can 1-D model replicate realistic particle heat up?

Previous work[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.[1]

FEM simulation of detailed microstructural model with cell wall thermal properties

≈

FEM simulation of accurately shaped model with bulk thermal properties

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Low order/1-D heat transfer model appropriate shape descriptors and thermal properties

Images courtesy of Peter Ciesielski from NREL.

Low-order particle model

Approximate heat-up as 1-D conduction with bulk properties and simple boundary conditions.

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

intra-particle heat conduction

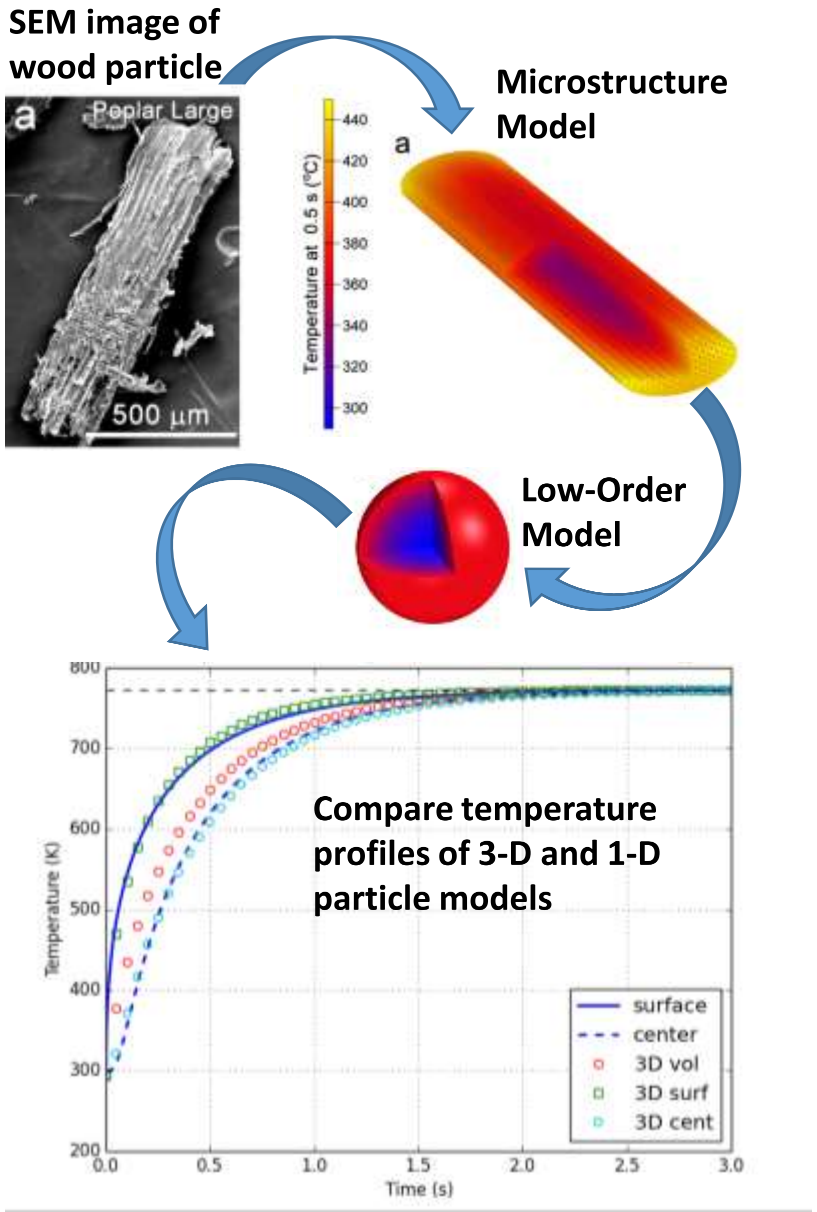
$$k\left.\frac{\partial T}{\partial r}\right|_{r=R} = h\left(T_\infty - T_R\right)$$

boundary condition with convection at particle surface

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0$$

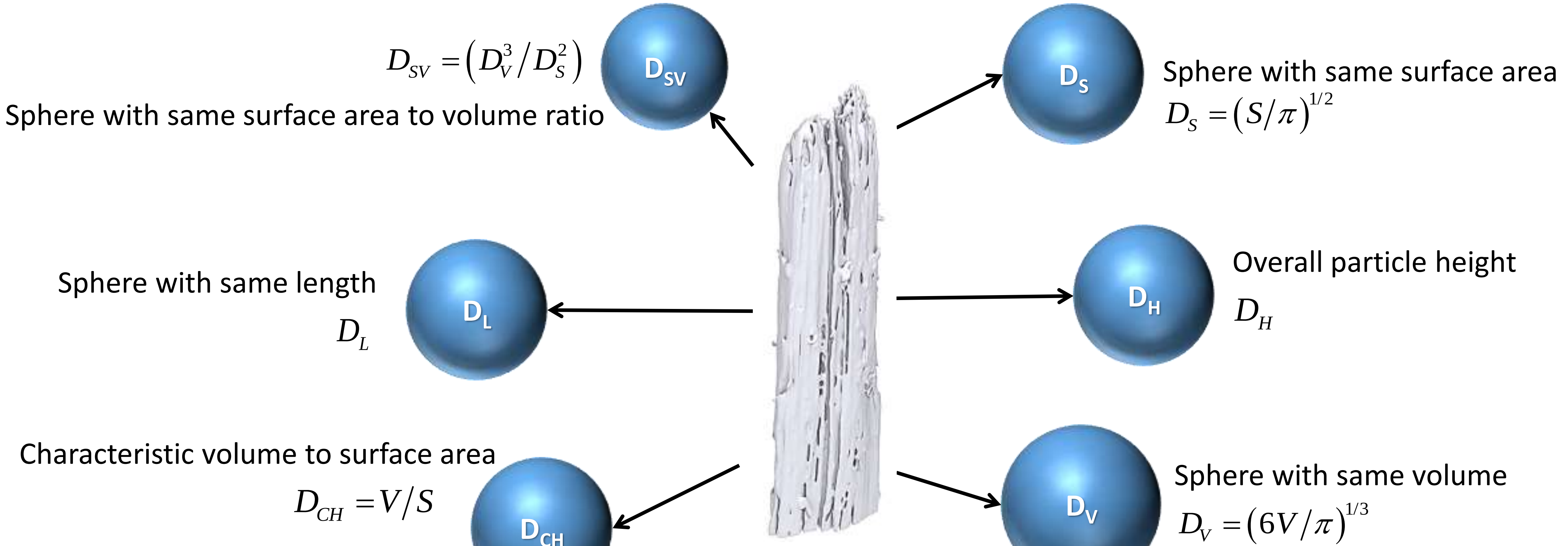
boundary condition with symmetry at particle center

Where
ρ = density (kg/m^3)
C_p = heat capacity (J / kg·K)
k = thermal conductivity (W / m·K)
T = temperature (K)
T_∞ = 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.

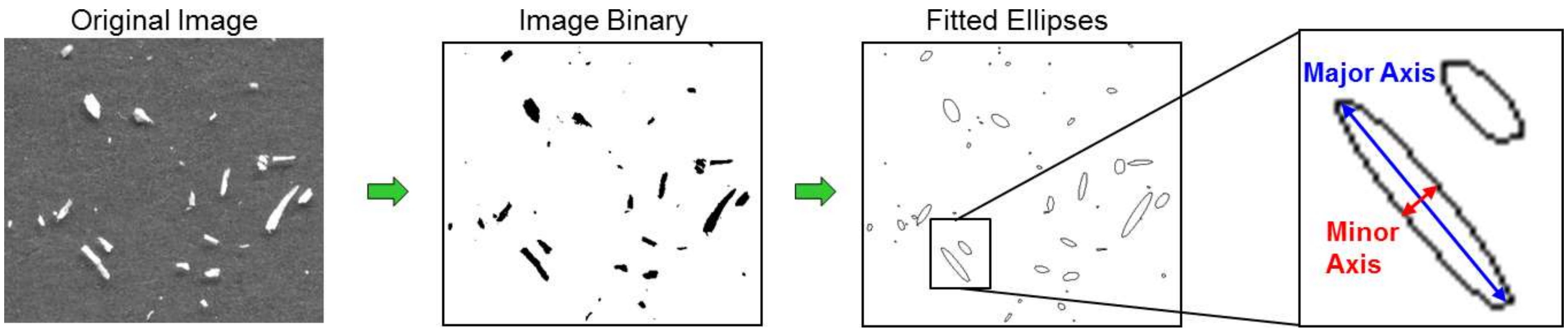


Irregular shaped wood particle

Particle size distribution determined from image analysis

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.



Source: Peter Ciesielski, NREL.

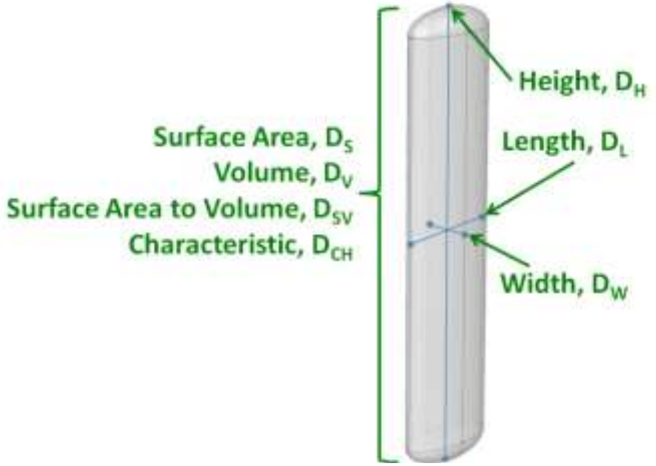
More details about particle characterization provided in microstructure paper.[1]

Dsv model reproduces 3-D temperature profiles

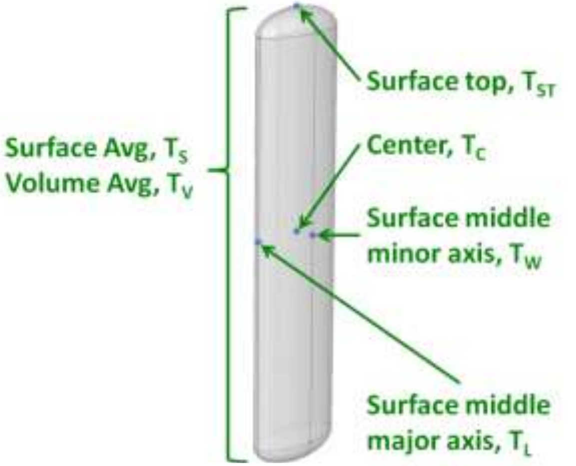
Bulk properties from Wood Handbook used for 3-D and 1-D particle model comparison for pure heat conduction (no kinetics).

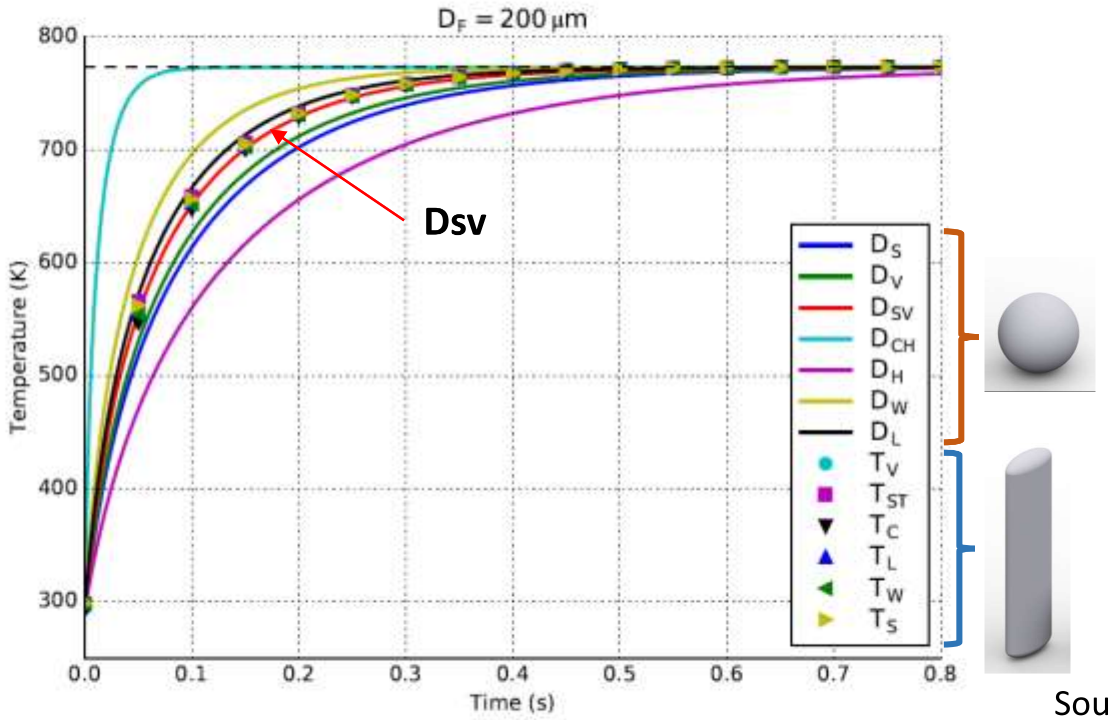
Property	Loblolly Pine	White Oak
ρ (kg/m^3)	540	720
k (W/m·K)	0.12	0.16
h (W/m^2·K)	350	350
C_p (J/kg·K)	103.1 + 3.867 T	103.1 + 3.867 T
T_o (K)	293	293
T_f (K)	773	773

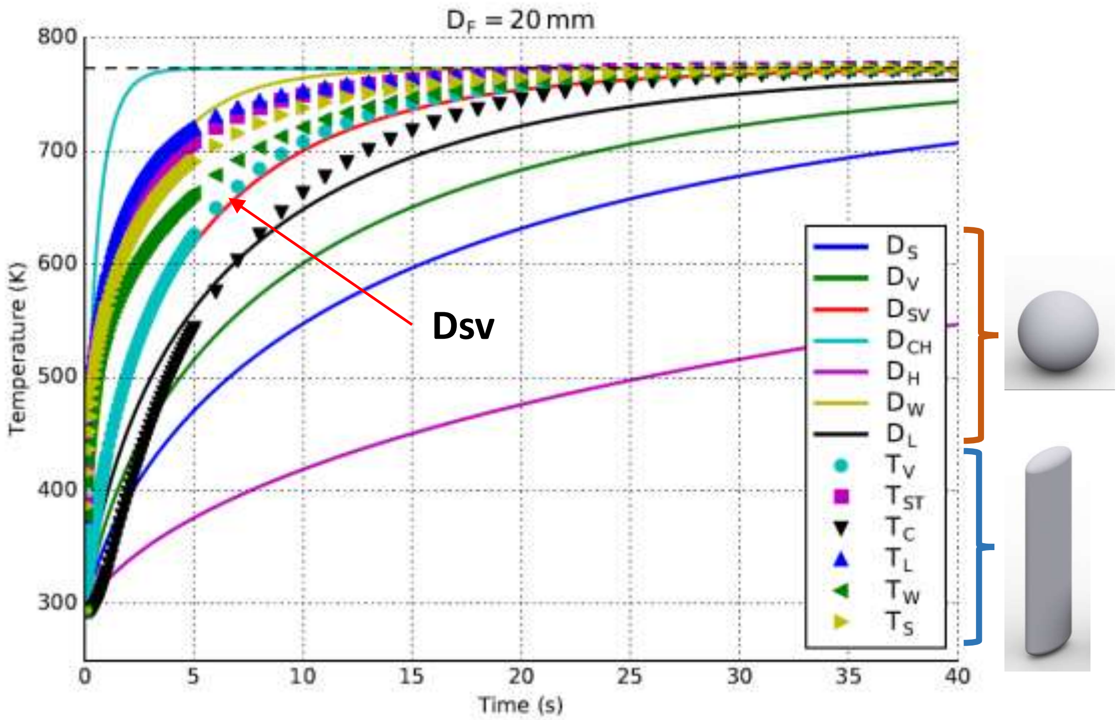
Geometry for calculating equivalent diameters.



Locations of temperature profiles.



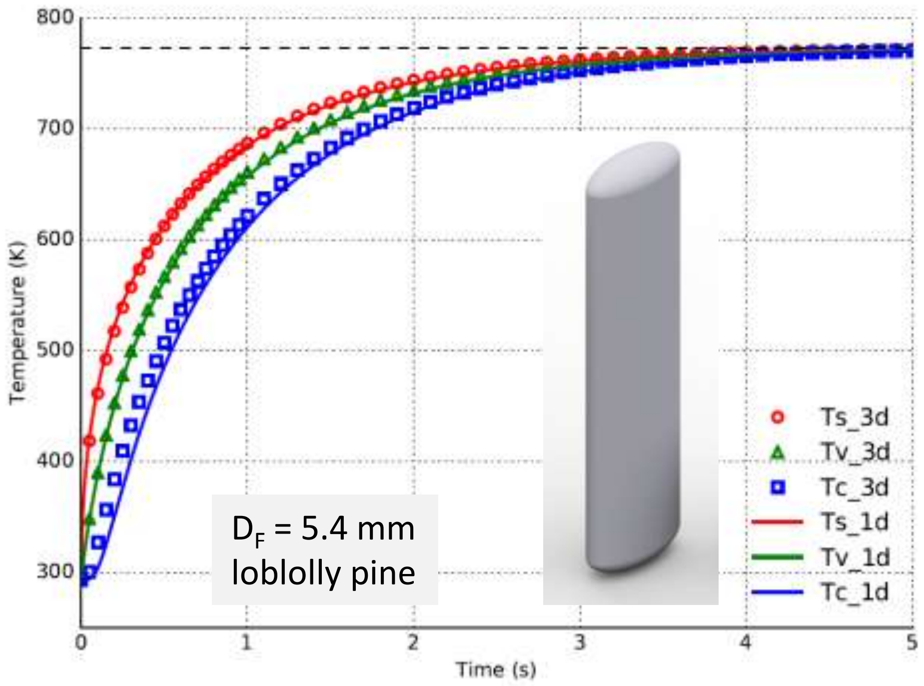


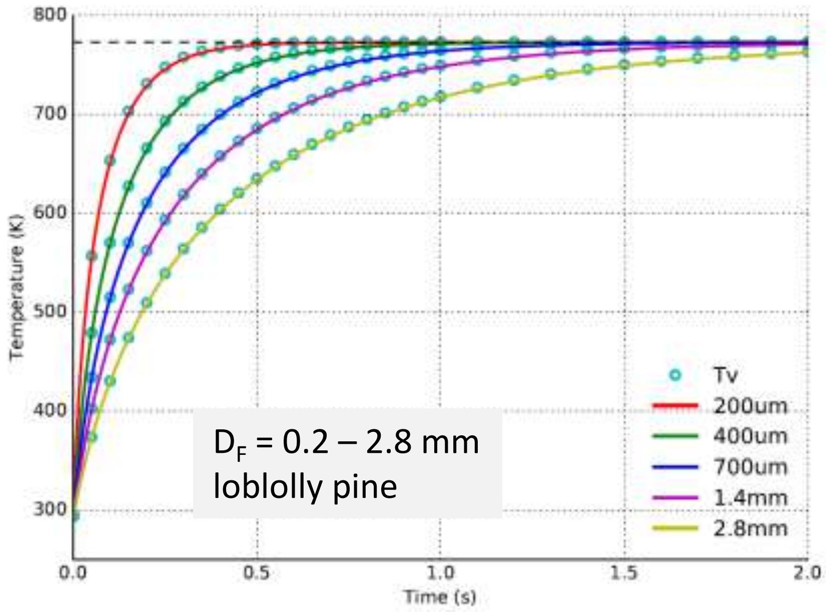


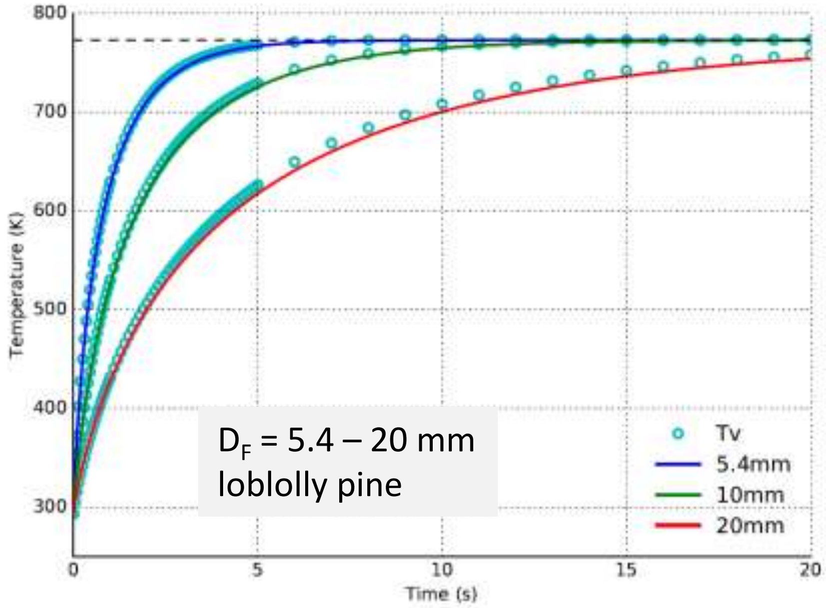
Source: [2].

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.





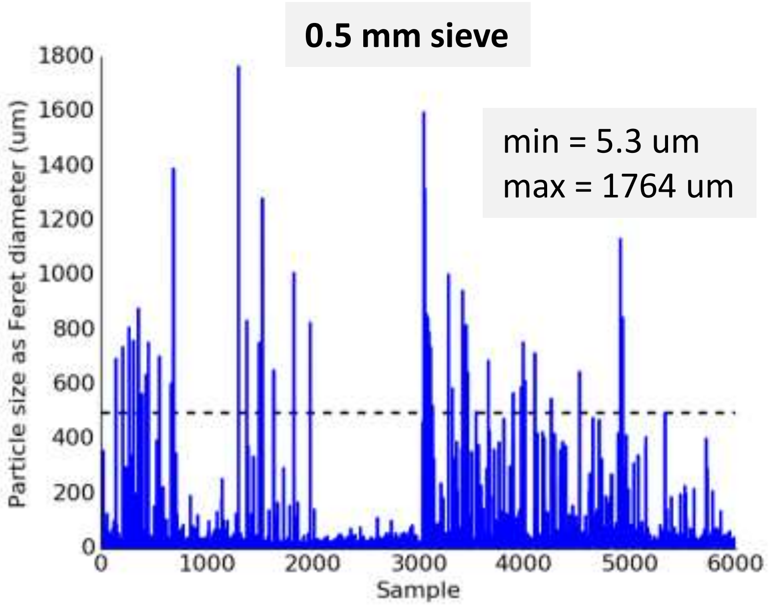


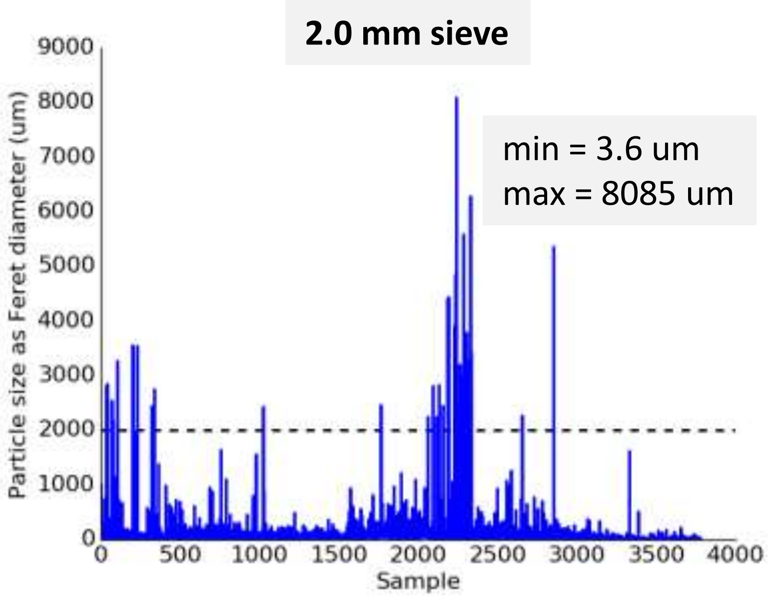
Volume average temperature of low-order Dsv particle model matches 3-D results for a range of particle sizes.

Source: [2].

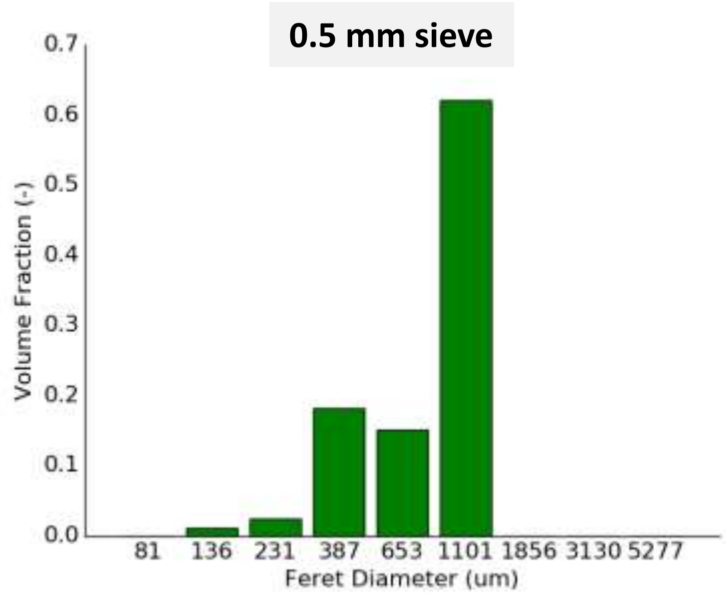
Biomass feedstock contains a range of particle sizes

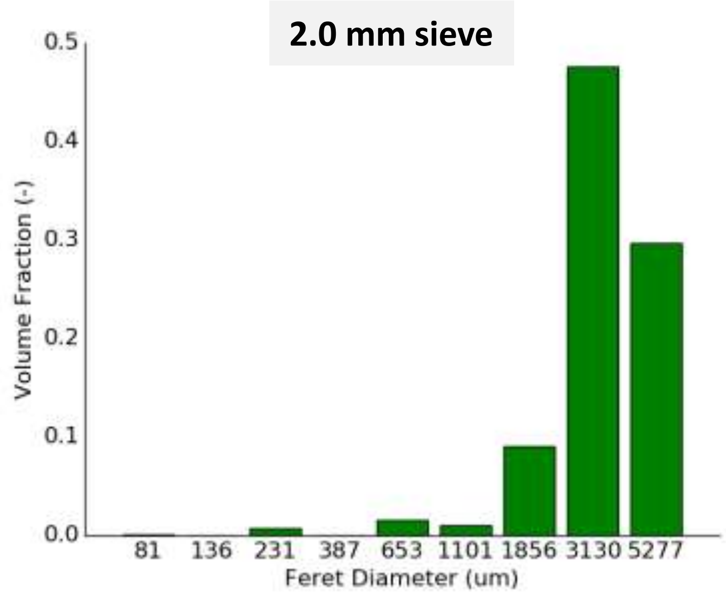
Raw data from image analysis





Particle size distribution from image analysis



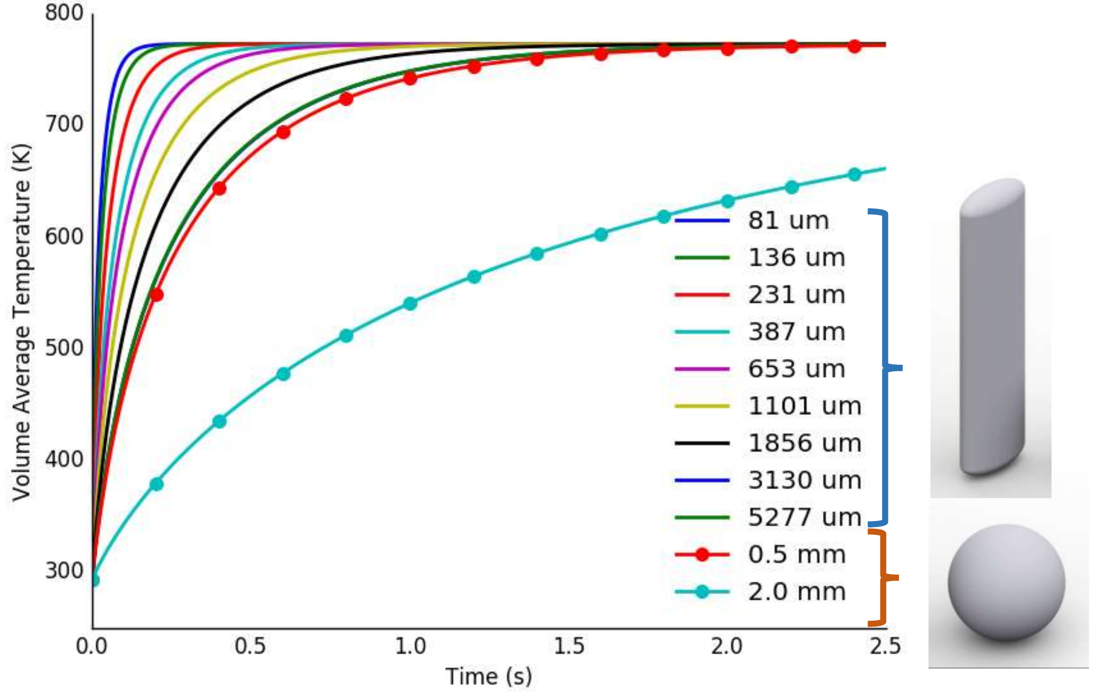


Particle characterization affects temperature profile

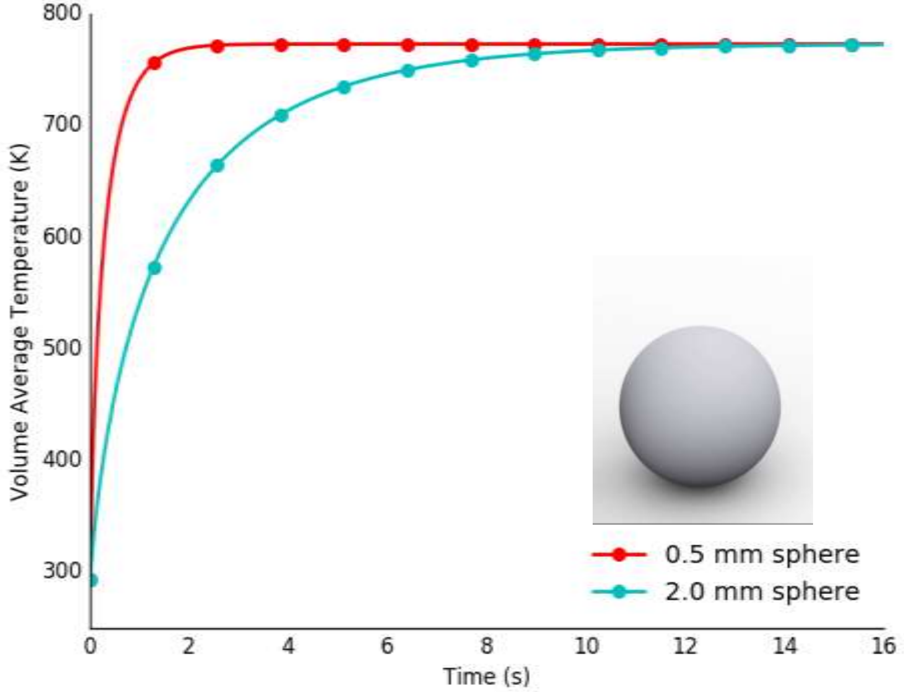
Low-order Dsv model utilizing bulk thermal properties for loblolly pine was applied to each particle size.

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.



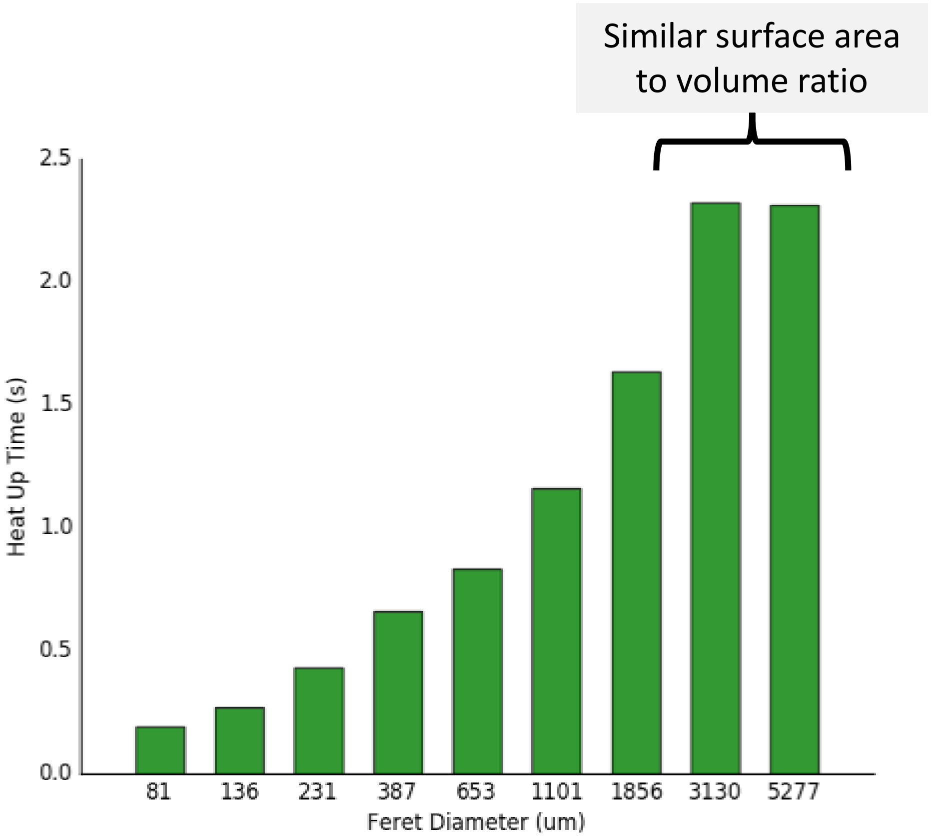
Temperature profiles from low-order model for solid sphere.

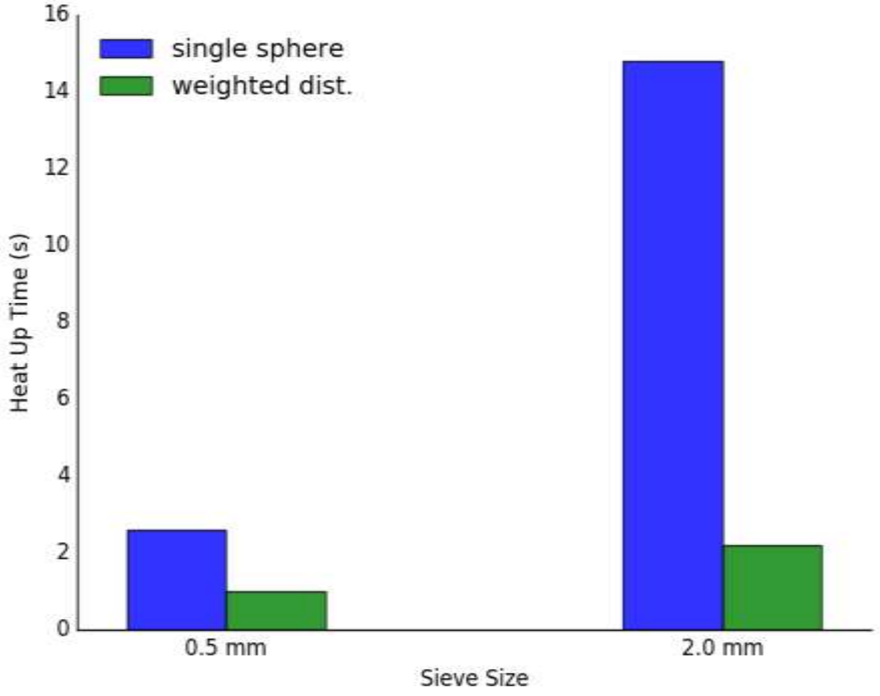


Particle size distribution affects overall heat up time

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.

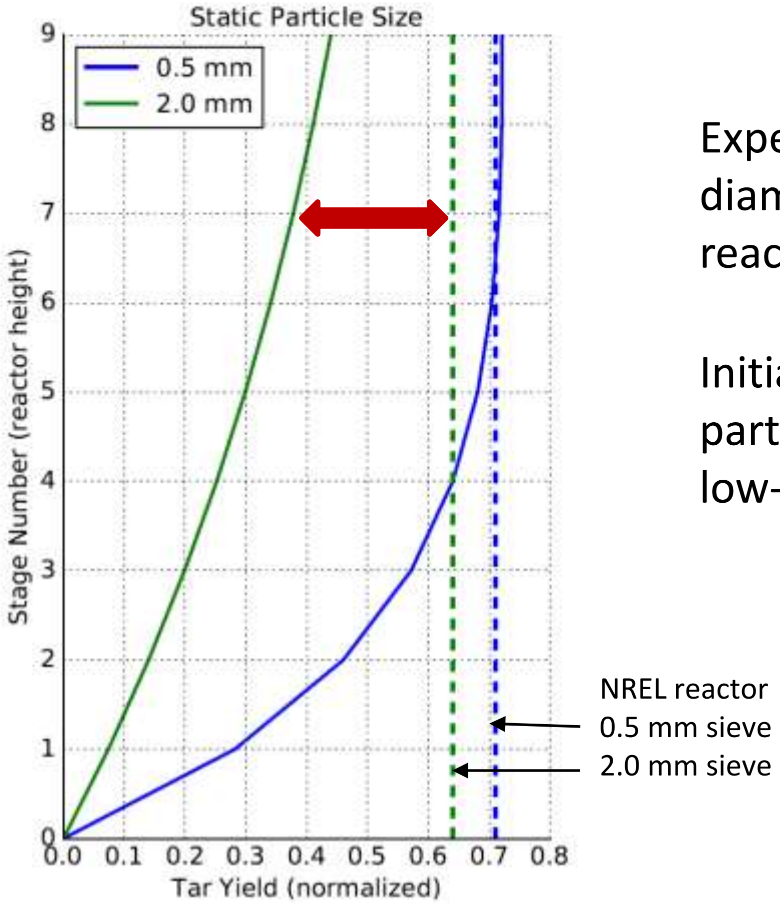




Reactor models must account for size distributions

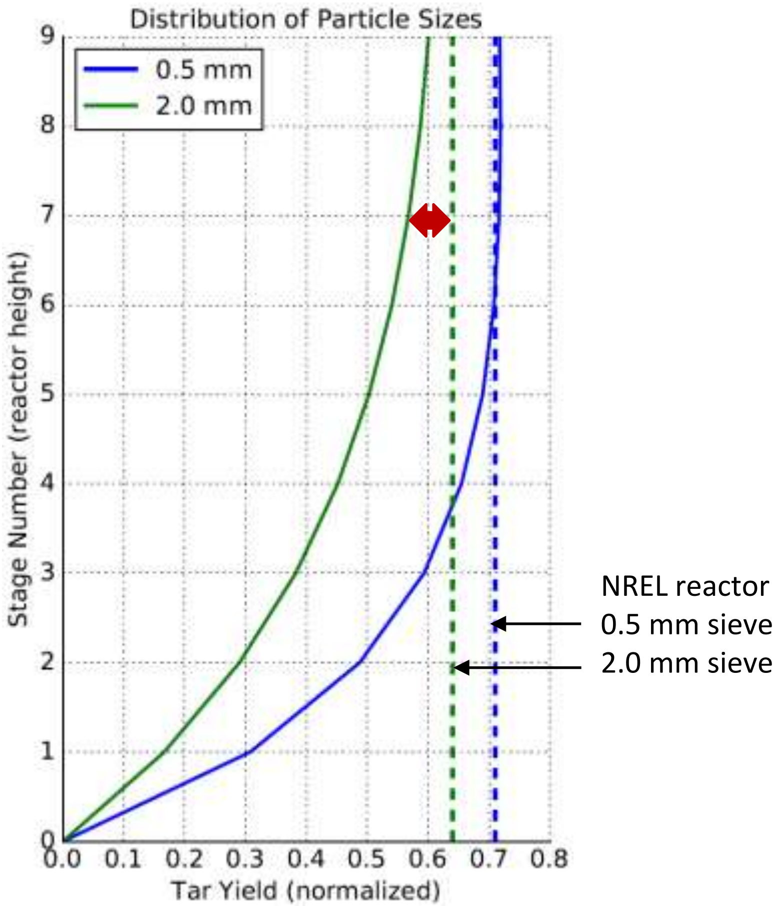
Products (wt. %)	0.5 mm sieve		2.0 mm sieve	
	Experiment	Model	Experiment	Model
Total liquids	**70.8 ± 1.1**	**72.1**	**63.5 ± 1.9**	**44.0**
Char	9.5 ± 0.1	13.7	11.7 ± 1.3	8.2
Gas	15.5 ± 0.6	12.3	18.7 ± 0.8	6.5

Products (wt. %)	0.5 mm sieve		2.0 mm sieve	
	Experiment	Model	Experiment	Model
Total liquids	**70.8 ± 1.1**	**72.1**	**63.5 ± 1.9**	**60.1**
Char	9.5 ± 0.1	13.7	11.7 ± 1.3	11.3
Gas	15.5 ± 0.6	12.3	18.7 ± 0.8	9.6



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

[1] Ciesielski, Peter N., Michael F. Crowley, Mark R. Nimlos, Aric W. Sanders, Gavin M. Wiggins, Dave Robichaud, Bryon S. Donohoe, and Thomas D. Foust. **Biomass particle models with realistic morphology and resolved microstructure for simulations of intraparticle transport phenomena**. *Energy & Fuels* 29, no. 1 (2014): 242-254.

[2] Wiggins, Gavin M., Peter N. Ciesielski, and C. Stuart Daw. **Low-Order Modeling of Internal Heat Transfer in Biomass Particle Pyrolysis**. *Energy & Fuels* 30, no. 6 (2016): 4960-4969.

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Supplemental Material

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