Mathematical Modeling of Biomass Pyrolysis Using Discrete Element Method

Mohera Narimetla

Advisor: Joseph J. Biernacki, Department of Chemical Engineering

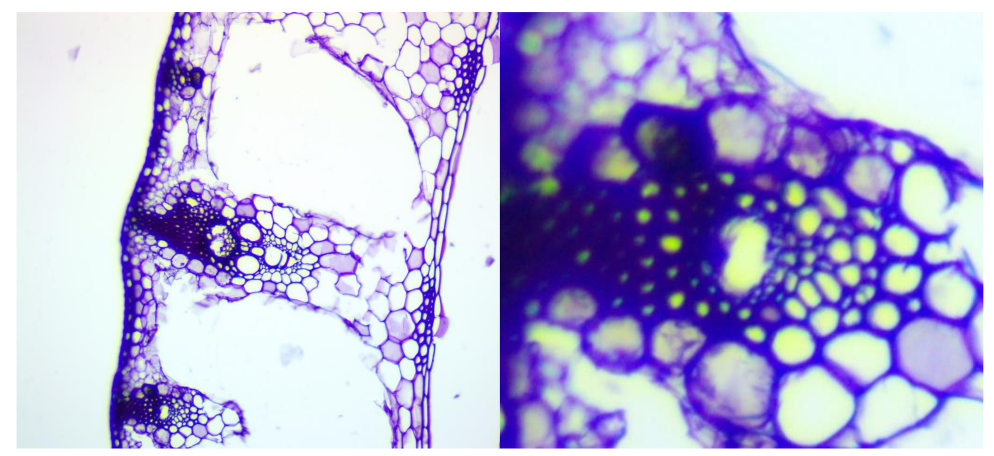
Introduction

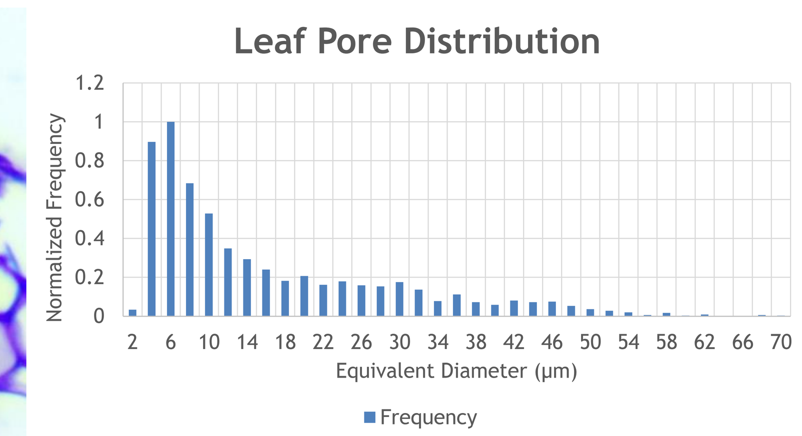
Biomass pyrolysis is the thermal decomposition of lignocellulosic matter in the absence of oxygen. The products of this process are bio-oils, bio-gases, and bio-char - sustainable, non-fossil carbon resources. To better understand pyrolysis and optimize the design of pyrolysis reactors, mathematical modeling of chemical and physical (microstructural) changes induced by pyrolysis is much needed.

Discrete Element Method - Application

Although various pyrolysis models have been developed, most involve continuum-based strategies with limited ability to model physical change. The present work, however, utilizes a discrete element method (DEM) which models the structure as “discrete” individual particles. As can be seen here, plant-based biomass is made up of cellular structures that closely resemble circles in a cross-section. This makes the DEM approach easily applicable to biomass.

Physical Images and Data





Figures 1-3: (1,2) Cross-sectional images of switchgrass leaf and (3) Leaf pore size distribution by Rachael Koehler

Mathematical Model

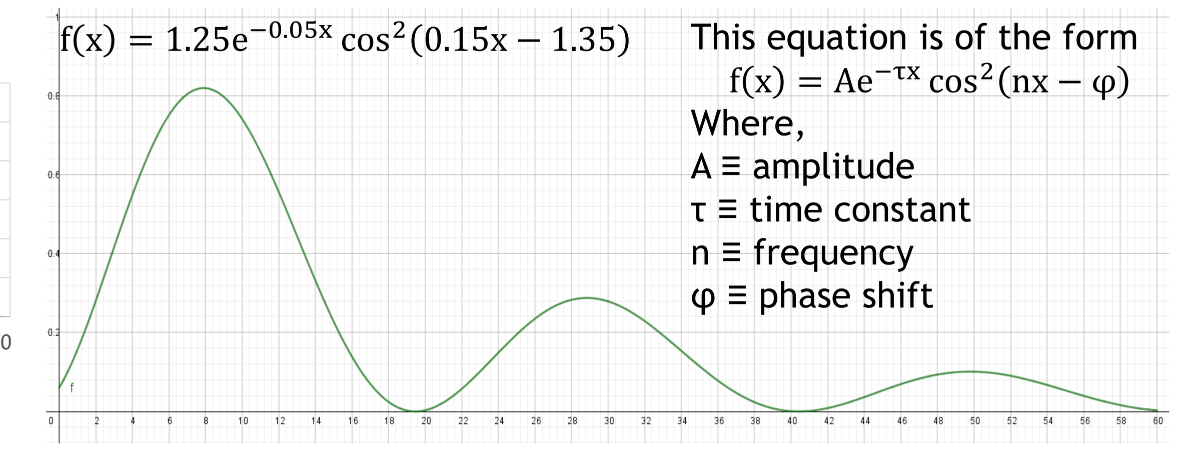


Figure 4: Probability density function (PDF) of size distribution

Simulated Distribution

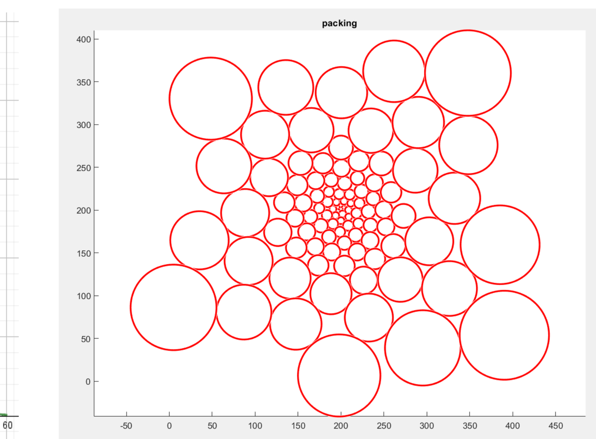


Figure 5: Visual distribution of 100 particles from PDF

Results - Shrinkage

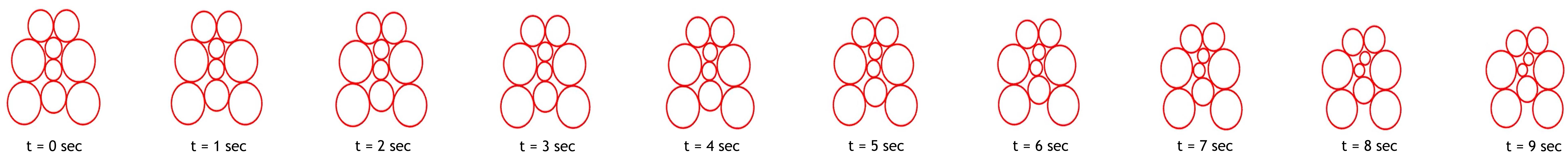


Figure 6: Mathematical model of pyrolysis-induced shrinkage over time span of nine seconds for nine particles

Methods

Steps in Model Development

Step 1: Modeled a two-mass system with hard repulsive forces

Step 2: Extended model to n particles

Step 3: Calculated Hamiltonian for validation purposes

Step 4: Imposed a soft interparticle attractive force to make ensemble behave like a solid

Step 5: Implemented chemical kinetics and tied particle size to reaction extent

Step 6: Developed particle ensemble that mimics biomass using a probability density function

Graphs and Calculations

Forces

Wall Force: $\frac{F_w}{(x_i - r)^2}, i \in \{1,2,\ldots,n\}$

Hard Repulsive Force: $F_R = \frac{F_p}{(d - 2r)^2}$

Soft Interparticle Force: $F_{spring} = k_{spring}(d - 2r)$

Zero-Order Shrinkage Kinetics

$$m_i = \rho_i\left(\frac{4}{3}\pi r_i^3\right) \quad \frac{dm_i}{dt} = -k$$

$$\Rightarrow r_i = \sqrt[3]{\frac{3}{4\pi}\frac{m_i}{\rho_i}} \quad \Rightarrow \frac{dm_i}{dt} = 4\pi\rho_i r_i^2\frac{dr_i}{dt} = -k$$

$$\Rightarrow \frac{dr_i}{dt} = \frac{-k}{4\pi\rho_i r_i^2}$$

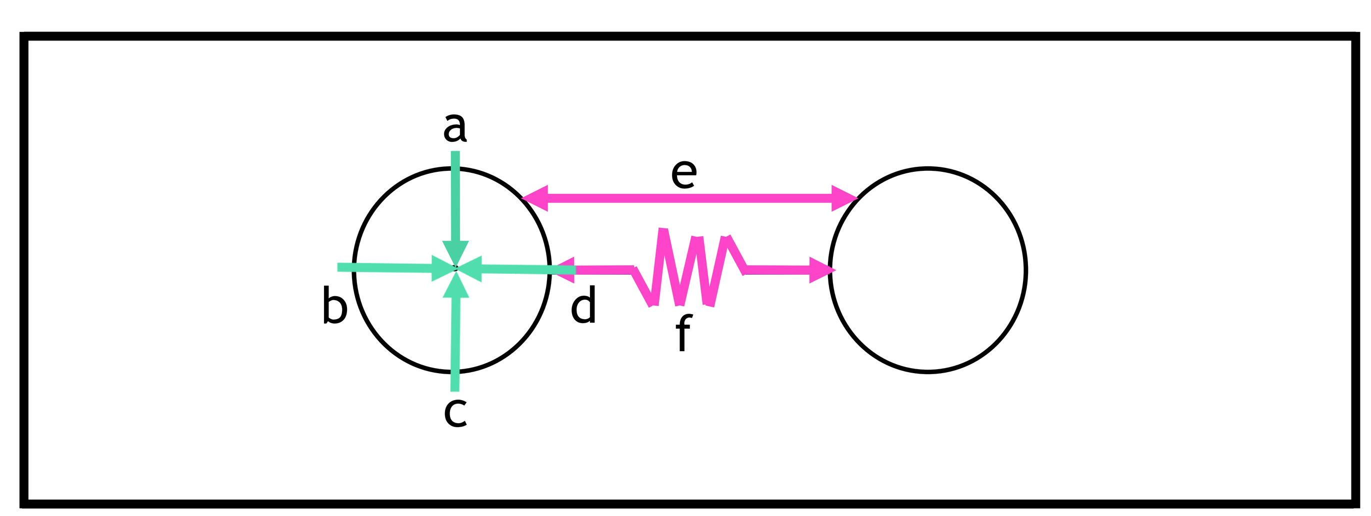


Figure 7: (a) Top wall force (b) Left wall force (c) Bottom wall force (d) Right wall force (e) Hard repulsive force (f) Soft interparticle force

Conclusions

In comparing the mathematically simulated models to the physical microstructure of switchgrass, it is clear that the implementation of DEM serves as a viable option for accurately representing pyrolysis-induced shrinkage. In order to further upscale the model to depict the behavior of the entire microstructure, further work must be conducted, including implementation of specific particle locations and additional research into the microstructure of switchgrass to apply appropriate kinetics.

References

Thornton, Colin. *Granular Dynamics, Contact Mechanics and Particle System Simulations: A DEM Study*. Springer International, 2016.

Adenson, Michael O., *Fuel*, Elsevier, 31 Aug. 2017.

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