Using Python to Model Biomass Pyrolysis Reactors

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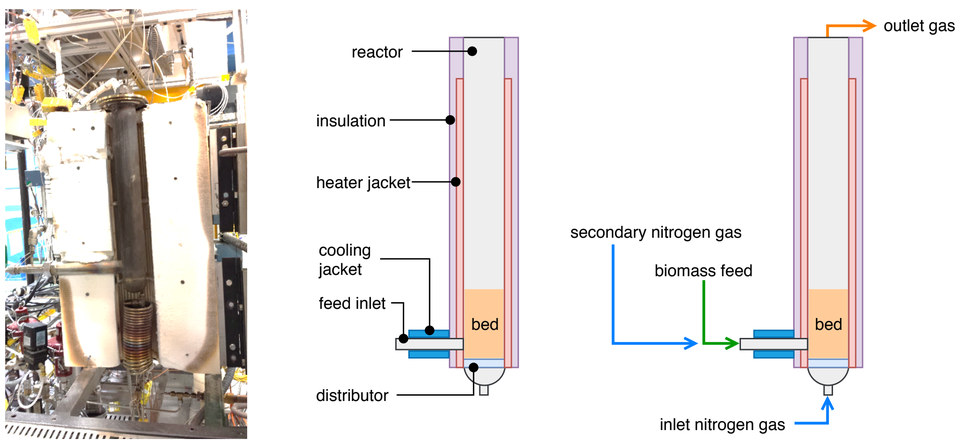
Background

Fast pyrolysis is a leading candidate technology for the thermochemical conversion of solid biomass into liquid bio-oil which can be used for biofuel and high-value chemical production.

Bio-oil is commonly generated in fluidized, circulating, or entrained flow reactor systems in which biomass particles rapidly devolatilize in the absence of oxygen into mixtures of light gases, condensable bio-oil vapors, and solid char.

To maximize bio-oil yields, the reactor typically operates at 500°C and must maintain particle residence times in the range of 2 to 5 seconds and gas residence times less than 1 second. Optimal reactor design and control are crucial to achieving commercially viable products.

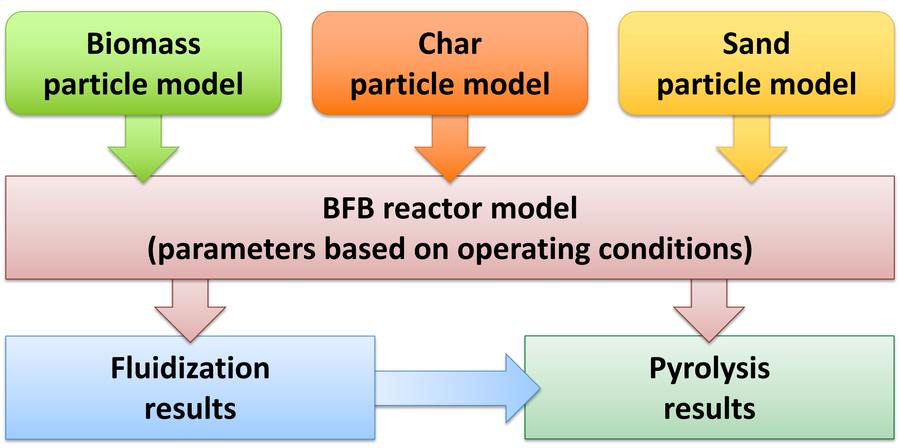


Left – BFB reactor at NREL. Right – reactor components and main process flows. Diameter 2.3 inches, height 17 inches.

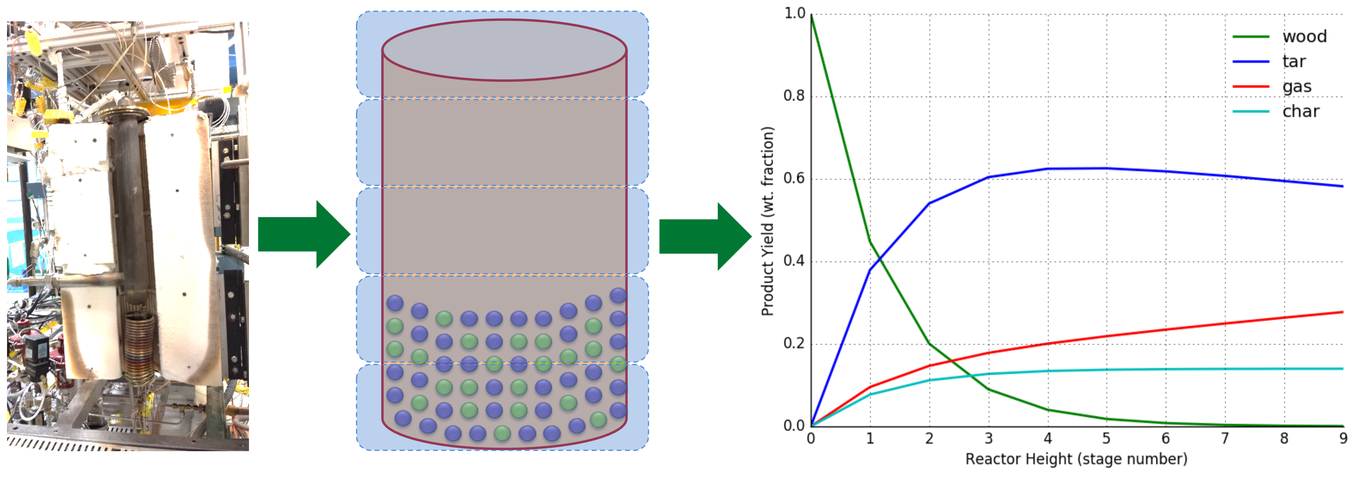
Bubbling fluidized bed (BFB) reactor

The purpose of this project is to develop a Pythonic approach for modeling biomass pyrolysis yields and fluidization conditions in BFB reactors with different residence time distributions.

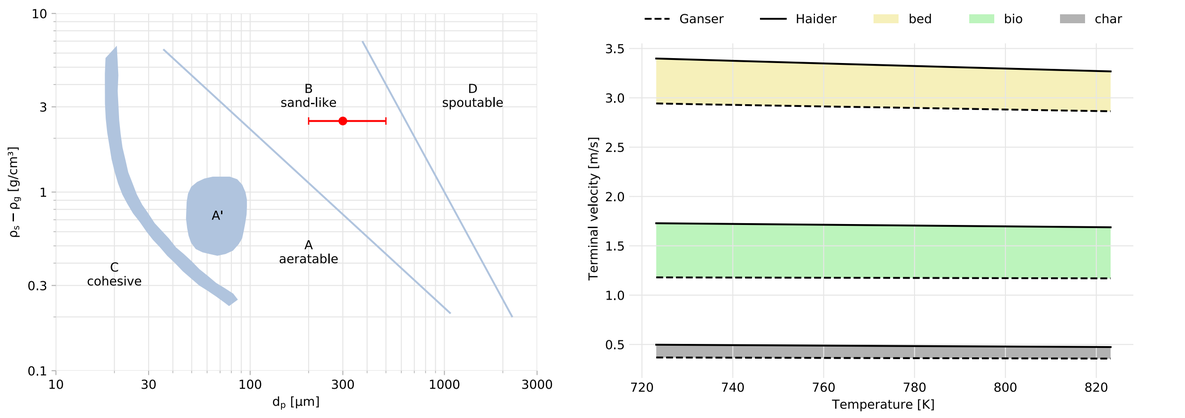
NumPy and **SciPy** are used extensively for solving systems of equations (PDEs and ODEs) and performing vectorized calculations relevant to the BFB model. **Matplotlib** is used for visualizing model results and experimental data.



Particle models represent biomass, char, and sand properties. The BFB reactor model uses particle properties and operating conditions to determine fluidization behavior and estimate pyrolysis products.



BFB reactor is represented as a series of CSTRs. Wood conversion to tar, gas, and char is estimated with the Liden 1988 kinetics scheme at 500°C.

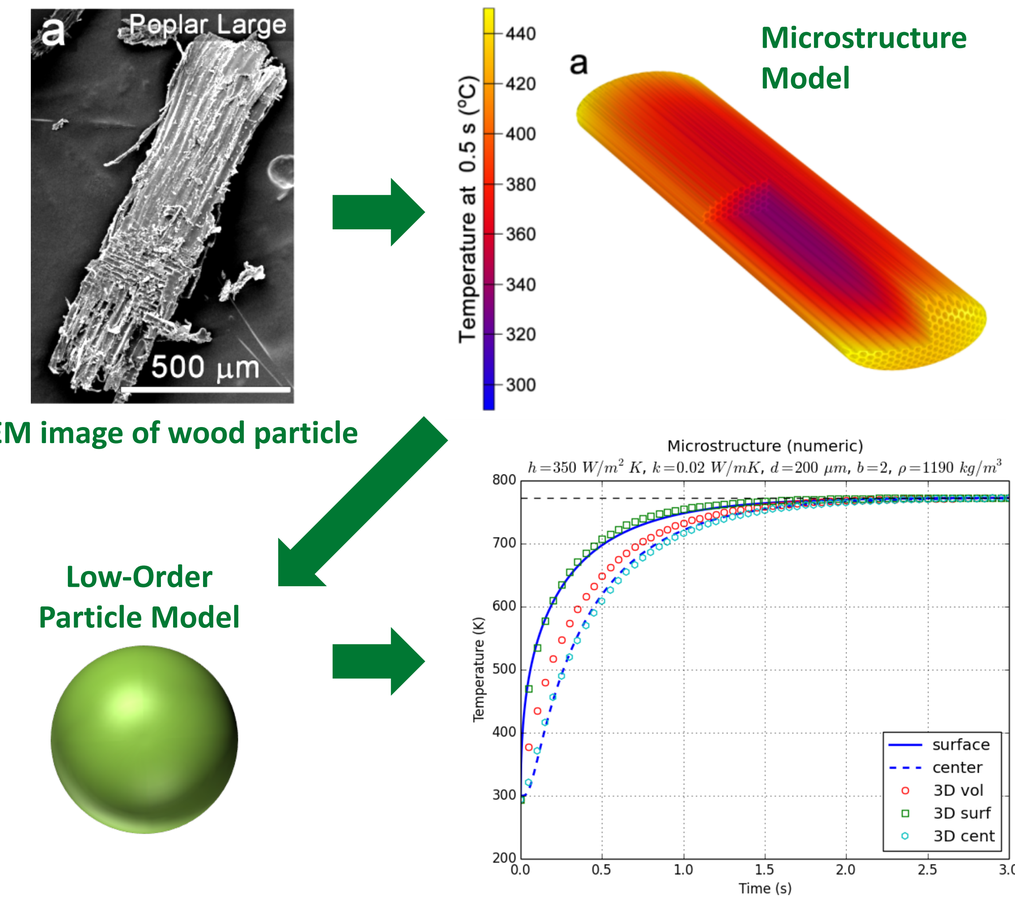


Left – Geldart chart for particle classification. X-axis is particle diameter and Y-axis is relative fluidizing density. Red bar represents bed particle size distribution in NREL reactor. Right – terminal velocity of bed, biomass, and char particles using equations from Ganser 1993 and Haider 1989.

Intra-particle heat conduction in biomass

As part of the reactor model, a particle model accounts for the anisotropic and aspherical characteristics of biomass particles. The model utilizes intra-particle heat conduction to estimate the extent of pyrolysis within a wood particle.

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



The particle model implements an equivalent spherical diameter and averaged values for wood thermal properties to reasonably predict the internal temperature profile of a realistic wood particle. SEM image and 3D Comsol simulation from Peter Ciesielski et al. at NREL.

Chemics package and CCPC code

Chemics is a collection of Python functions for chemical reactor engineering. See documentation https://chemics.github.io and main repository https://github.com/chemics for more details. Contributions from the Python community are welcome.

Python code for the BFB reactor model and other CCPC related projects is available at https://github.com/ccpcode

Acknowledgment

The author would like to thank the U.S. DOE Bioenergy Technologies Office and program managers Kevin Craig, Jeremy Leong, and Trevor Smith. This work is part of the Consortium for Computational Physics and Chemistry (CCPC). Visit https://www.cpcbiomass.org for more information.