Simulation & AI for the Circular Economy of Bioenergy & Bioproducts

Background

- The concept of a biorefinery for the conversion of lignocellulosic biomass into the biofuel ethanol has existed for nearly 100 years.
- Molecular modeling of biomass for biofuels and bioproduct development has experienced substantial growth over the nearly two decades.
- Work exploring the application of machine learning and AI to further accelerate biomass processing and upgrading is now substantial and growing.

Approach

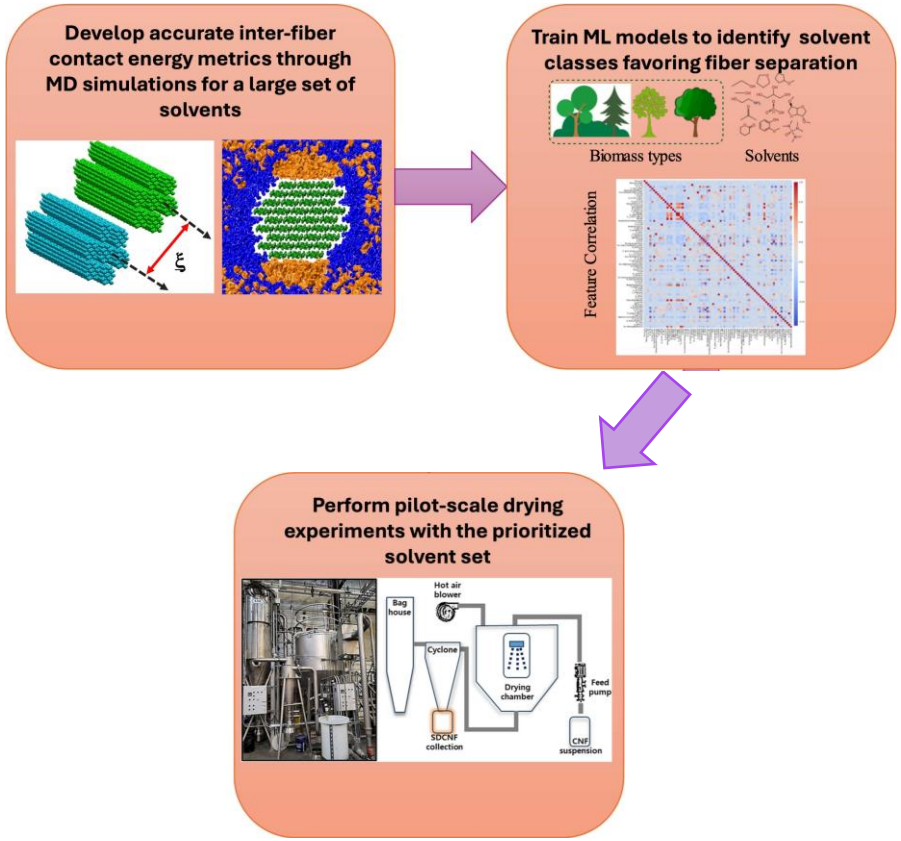
- An exhaustive literature review was performed that summarizes the role of molecular simulations and the growth of AI/ML approaches in the elucidation of biomass deconstruction and polymer-based upgrading.

Key Observations

- Molecular simulation approaches have discovered fundamental driving forces underpinning of biomass deconstruction under various conditions; however, future work will likely require multi-scaled approaches that bridge spatial scales associated with chemical reactions.
- AI is quickly taking root and has made decisive advances. Key remaining challenges are a lack of available high-quality comprehensive datasets and the optimization of machine-learning features.

Significance

- AI-based models trained with data combined from MD simulation, quantum chemistry, and experiment can optimize simulation parameters, enhance the interpretability of computed results, and uncover complex structure-property relationships. This will usher in a paradigm change in biomass pretreatment and bio-product upgrading.



An example MD/ML pipeline for material and solvent discovery.

Smith et al (2025). "Molecular simulation and artificial intelligence for the circular economy of bioenergy and bioproducts" *Biophys. J.,*
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