Polymer Principles Behind Solubilizing Lignin With Organic Cosolvents for Bioenergy

Objective:

- Obtain a predictive understanding of lignin solvation in mixtures of water with polar aprotic solvents. This knowledge will help overcome the challenges posed in valorizing lignin by its chemical complexity.

Approach:

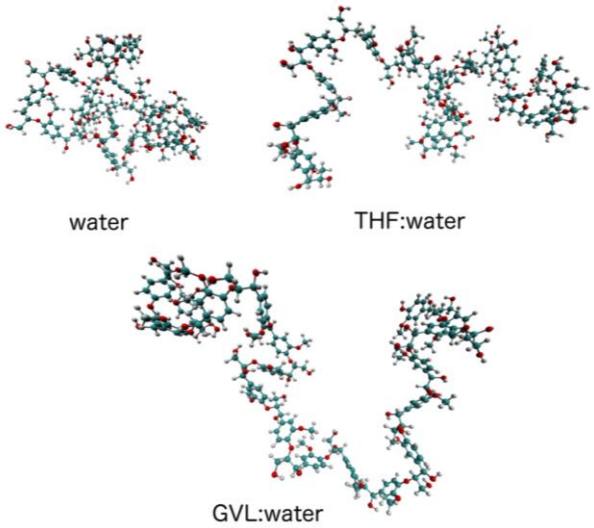
- Investigate the conformations of model lignin polymers in two mixtures of tetrahydrofuran (THF):water and γ-valerolactone (GVL):water using molecular dynamics simulations.

Results:

- A well-established theory of self-avoiding polymers in a "good" solvent describes accurately the physical conformations of all types of lignin in both solvent mixtures.
- The reduction in the lignin radius of gyration due to branching is accurately described by the Zimm-Stockmayer theory for both solvent mixtures.
- As the degree of methoxy substitution increases, the lignin radius of gyration does not change in THF:water, while it increases in GVL:water.

Significance:

- We validated the broad applicability of polymer physics concepts to lignin. These physico-chemical concepts will aid the development of effective techniques for converting lignin to valuable bioproducts.



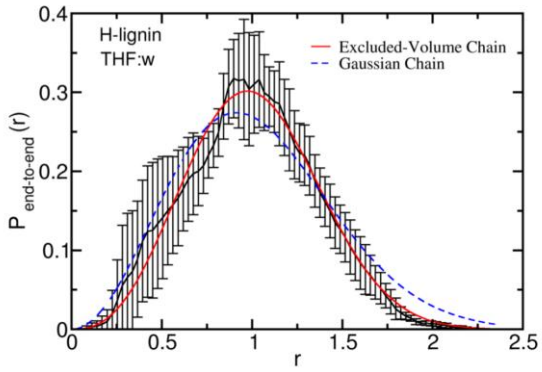


Figure. TOP: Molecular models of lignin in three solvents. BOTTOM: Fits of self avoiding polymer theory to MD data of the probability distribution of the lignin end-to-end distance.

Vural et al, *Green Chemistry*. 2020 Supported by the Biofuels SFA (ORNL and UTK)