

Segregation of Organosolv Solvents at the Cellulose Interface Influences Water Dynamics and Cellulose Deconstruction

Objective:

- Determine how common water-organosolv cosolvent systems interact with cellulose, which is key to understanding cellulose solubilization in biomass pretreatment for bioenergy and bioproducts

Approach:

- The first extensive molecular dynamics simulation study of how four organosolv-water mixtures – acetone, ethanol, tetrahydrofuran (THF) and γ -valerolactone (GVL) – behave on cellulose fiber surfaces.

Results:

- We find that qualitative differences exist in the distributions of the cosolvent components at the cellulose surface, with THF-, GVL- (and to a lesser extent) ethanol-water systems phase-separating.
- Median water-cellulose contact lifetimes increase for the cosolvent systems in the order of THF > acetone > ethanol > GVL
- In THF-water, unlike GVL-, acetone- and ethanol-water cosolvents, a significant fraction of surface water is slowed.

Significance:

- The surface phase separation and surface-water slowing may be of importance in enhancing reactions breaking down cellulose.

BER Biofuels SFA at ORNL (Dynamic Visualization of Lignocellulose Degradation ...)

Smith, M. D.; Cheng, X.; Petridis, L.; Mostofian, B.; Smith, J. C., Organosolv-Water Cosolvent Phase Separation on Cellulose and its Influence on the Physical Deconstruction of Cellulose: A Molecular Dynamics Analysis. *Scientific Reports* **2017**, 7 (1), 14494.

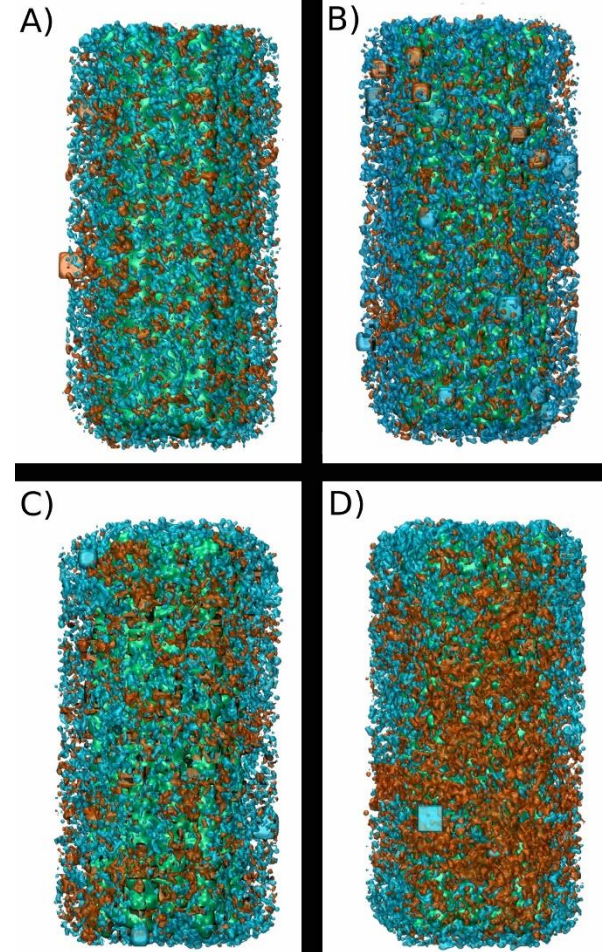


Figure: Two dimensional spatial density profiles of organosolv co-solvents on a cellulose surface. A) acetone, B) ethanol, C) GVL, D) THF. Orange colours indicate the organosolv, cyan/blue water and green cellulose. THF shows the most enhanced local segregation.