THF-Water solvation influences xylan hydrolysis rate and subsequent furfural product formation

Objective:

- Elucidate xylan behavior under THF-Water cosolvent used during co-solvent enhanced lignocellulosic fractionation (CELF).

Approach:

- We paired molecular simulation and experimental evidence, and revealed how the solvation of xylan in an water–tetrahydrofuran (THF) pretreatment can lead to single-pot conversion of biomass xylose to furfural and cellulose to 5-hydroxymethylfurfural.

Results:

- Xylan is solvated by both THF and water at CELF pretreatment temperatures.
- Partial solvation by THF was found to slow down xylan solubilization.

Significance:

- In aqueous solution, xylan is depolymerized faster than cellulose is, making it difficult to convert both biopolymers to fuel precursors at the same time.
- We showed that solvation by THF:water (CELF) slows the rate of xylan hydrolysis, allowing an economically desirable “single-pot” conversion of both xylan and cellulose to fuels and products.

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(Dynamic Visualization of Lignocellulose degradation …)

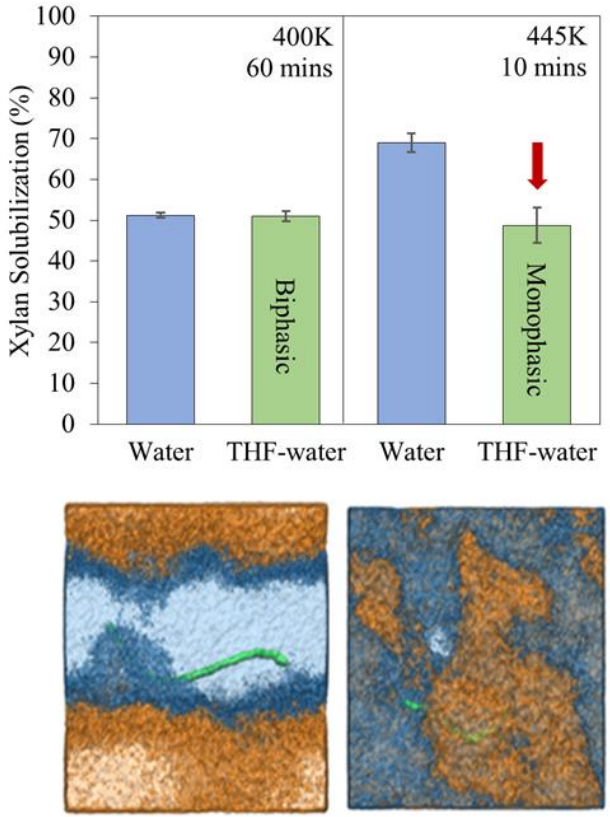

Figure: (Top) Experimental xylan solubilization under CELF (THF-water) or pure water conditions. (Bottom) Computational model of xylan hydration in biphasic and monophasic solvent states. Xylan (green), THF(orange), water(blue)

M.D. Smith et al. “Temperature-dependent phase behaviour of tetrahydrofuran-water alters solubilization of xylan to improve co-production of furfurals from lignocellulosic biomass.” *Green Chem*. 2018, 20(7): 1612-1920. DOI: 10.1039/c7gc03608f

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