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Wednesday, January 25th, 2023 at 4:00pm EST
Virtual Meeting: Zoom

Dr. Nicholas E. Thornburg, Ph.D.

Center for Integrated Mobility Sciences
National Renewable Energy Laboratory

Reaction engineering *in planta*? Tales of mass transfer limitations and their catalytic consequences at the mesoscale for next-generation biorefining

Between the molecular and reactor scales—familiar favorites to the chemical engineering community—lies an intermediate regime termed the "mesoscale" where chemical reaction kinetics and transport phenomena compete along similar time and length scales. However, little is known about the coupled chemistry and physics of biomass conversion at the mesoscale. These entangled phenomena govern effective rates of organic component extraction from plant cell walls during biorefinery feed fractionation processes, and often also during "one-pot" catalytic transformations. First, I will introduce an experimentally validated simulation framework that determines transport-independent kinetic rate constants upon incorporating realistic feedstock characteristics for an exemplary process that combines hardwood solvolysis and reduction catalysis. This generalizable mesoscale reaction–diffusion modeling approach will then be extended to validate and predict the alkaline deacetylation of corn stover, an emerging biorefinery pretreatment method that removes

acetyl from hemicellulose prior to mechanical refining to improve downstream enzymatic sugar yields. Reaction–diffusion models are developed and validated for three major anatomical fractions (cobs, husks and stalks), and model findings categorize experimental feedstock performance into kinetic-controlled vs. diffusion-controlled regimes based on the particle size and microstructural attributes of each tissue type. Critically, the model predicts that typical corn stover particles as small as ~2.3 mm in length are entirely diffusion-limited for acetate extraction, with experimental effectiveness factors calculated to be 0.50 for such processes. Overall, this presentation highlights opportunities to improve biomass fractionation and catalytic conversion via reaction engineering and provides actionable kinetic information to guide the design and scale-up of emerging biorefinery strategies.

Speaker Bio

Dr. Nicholas (Nick) Thornburg is a chemical reaction engineer in the Fuels and Combustion Science group within the Center for Integrated Mobility Sciences (CIMS) at the National Renewable Energy Laboratory (NREL). Nick joined CIMS in April 2020 and began his current role as a staff research engineer in October of the same year. He originally joined NREL's National Bioenergy Center (NBC) as a postdoctoral researcher in April 2017, where he studied particle-scale reaction engineering and multiphase chemical reactor design and optimization for biomass deconstruction. Nick's current research interests lie in multiphase reaction engineering for on- and off-board hydrogen carrier reforming and for the renewable synthesis of small-molecule chemicals and fuels, such as ammonia. Nick has a Bachelor of Science in Chemical Engineering from Washington University St. Louis and a Doctorate in Chemical Engineering from Northwestern University. His doctoral research at Northwestern focused on understanding heterogeneous transition metal oxide catalysts for applications in sustainable chemical manufacturing, work which was sponsored by The Dow Chemical Company. Before joining NREL, Nick gained industrial research and development experience with 3M.

Please refer to email announcement for login details.

Presentation	**4:00 PM**	**Annual Membership Dues**	**$35 (*Students* = $15)**

Deadline for reservations is **4:00PM Monday, January 23rd, 2023**

To make your reservation, fill out the online form.