Department of Chemical
and Biological Engineering
UNIVERSITY OF WISCONSIN–MADISON

2020 Fall CBE Seminar Series

presents:

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Next-generation Mechanistic Modeling Techniques for Complex Catalytic Reaction Networks

Several catalytic processes tend to be complex in that the underlying reaction system comprises of several hundred to thousands of species and reactions. Building and analyzing such reaction networks manually is cumbersome and error-prone. Further, developing detailed mechanistic models, as is done routinely for small reaction systems, is computationally intractable. Research in my group focuses on developing scalable techniques to study such complex reaction networks.

In this talk, I will present a rule-based computational tool, Rule Input Network Generator (RING), to construct and analyze the mechanism of such complex reaction networks. RING can construct an exhaustive network of all plausible reactions and species of a system and identify reaction pathways forming a specific product through rule-based queries and "prune" out energetically infeasible pathways. Using polyol conversion as an example of a complex reaction network seen in biomass conversion, I will demonstrate how RING can be used, in a near-automated fashion, to obtain compact microkinetic models that are consistent with experiments.

Tuesday, Dec. 1, 2020

Lecture at 4:00 p.m.

https://uwmadison.zoom.us/j/91376473708