Northeastern University
College *of* Engineering

Please join us for a
Special Chemical Engineering & Bioengineering Seminar

Wednesday, January 23, 2013
108 West Village H
11:45 a.m. – 1:00 p.m.

"Designing Reaction Pathways to Novel Chemicals and Materials Using Kinetic Modeling"

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ABSTRACT

Reaction pathway analysis is a powerful tool to design routes to chemicals and materials that are novel and lead to materials with unique and tailored properties. We have developed methods for the assembly of kinetic models of substantive detail that enable the atomic scale to be linked with the process scale. We have applied our methodology to a wide range of problems, including production of silicon nanoparticles, biochemical transformations, polymerization and depolymerization, and tropospheric ozone formation. While the chemistries we have studied are seemingly very disparate, applying a common methodology to study them reveals that there are many features of complex reaction networks that are ubiquitous.

The first portion of the talk will focus on our mechanistic understanding of the competing reactions in fast pyrolysis of cellulose and other glucose-based carbohydrates through a unified microkinetic model. The model incorporates the reactions of the cellulose chain and the glucose intermediate to form a variety of bio-oil components, which are confirmed by either experiments or theoretical calculations reported in the literature. The model yields of all the major primary fast pyrolysis products, matching well with the experimental data over the temperature range of 400–550 ^{o}C, and, utilizing the same set of rate coefficients, was able to predict the dominant products of fast pyrolysis of maltohexaose, cellobiose and glucose.

The second portion of the talk will focus on designing novel pathways for the sustainable microbial production of high-value organic compounds as an attractive alternative to organic syntheses that utilize petrochemical feedstocks. For example, the high cost of and the numerous applications for 3-hydroxypropanoate (3HP) make it a valuable target for biosynthesis. We applied the Biochemical Network Integrated Computational Explorer (BNICE) framework for the automated construction and evaluation of metabolic pathways to explore novel biosynthetic routes for the production of 3HP from pyruvate. Among the pathways to 3HP generated by the BNICE framework were numerous promising novel pathways.

The last part of the presentation will focus on the synthesis of gradient copolymers. Kinetic Monte Carlo (KMC) models, which track molecules instead of concentration, were developed in order to track the explicit sequence distribution for each copolymer chain. Nitroxide-mediated controlled radical polymerization (NM-CRP) was used in synthesizing S/AS and MMA/S gradient copolymers because of its pseudo-living property. The effects of different synthesis factors on the formation of the compositional gradient along copolymer chains will be described, and the ability to tailor the monomer-by-monomer sequence will be demonstrated.

BIOGRAPHY: Dr. Linda Broadbelt is Sarah Rebecca Roland Professor in and Chair of the Department of Chemical and Biological Engineering University at Northwestern University. She received her B.S. in chemical engineering from The Ohio State University and graduated *summa cum laude*. She completed her Ph.D. in chemical engineering at the University of Delaware in 1994 where she was a Du Pont Teaching Fellow in Engineering, a National Science Foundation Graduate Fellow, and a DuPont PhD in Engineering Fellow. At Northwestern, she was appointed the Donald and June Brewer Junior Professor from 1994-1996.

Refreshments will be served