

Chemical Engineering Seminars – HT 2007

Week 1: Tuesday 16 January, 4:15-5.15 pm
Lecture Room 2, Thom Building, Engineering Science

Creating and Harnessing Complex Reaction Networks

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Abstract

We have developed methods for automated generation of reaction mechanisms of complex systems that allow kinetic models of substantive detail to be built. Molecules are represented as graphs and matrices, and operations on these representations allow reaction to be carried out, molecule uniqueness to be determined, and properties to be calculated. We have applied our methodology to a wide range of different 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.

Bio-sketch

Prof. Broadbelt is Professor in the Department of Chemical 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 where she was a Du Pont Teaching Fellow in Engineering. At Northwestern, she was appointed the Donald and June Brewer Junior Professor from 1994-1996.

Her research and teaching interests are in the areas of multiscale modelling, complex kinetics modelling, environmental catalysis, novel biochemical pathways, and polymerization/depolymerization kinetics. One main research emphasis is computer generation of complex reaction mechanisms, and application areas include biochemical pathways, silicon nanoparticle production, and tropospheric ozone formation. Her honors include a CAREER Award from the National Science Foundation, appointment to the Defence Science Study Group of the Institute for Defence Analyses, and selection as the Ernest W. Thiele Lecturer at the University of Notre Dame and the Allan P. Colburn Lecturer at the University of Delaware.