ABSTRACT

Reaction pathway analysis and kinetic modeling are powerful tools to design novel routes to chemicals, identify optimal processing conditions, and suggest catalyst design strategies. We have developed methods for the assembly of kinetic models of substantive detail that link the atomic and process scales. We have applied our methodology to seemingly very disparate chemistries, yet applying a common methodology reveals that there are many ubiquitous features of complex reaction networks for chemical and biological systems. The first part of this talk will focus on mechanistic modeling of the conversion of hydrocarbons from renewable sources, from quantitative analysis of chemical catalysis by native inorganic constituents to mechanistic understanding of how enzymes achieve exquisite selectivity for similar conversion processes, leading to the potential for the design of novel (bio)chemical pathways. However, the design of novel pathways was carried out in the absence of any quantitative kinetic modeling, raising the intriguing question of whether data science approaches alone are sufficient to understand complex reaction networks. We demonstrate the application of data science methods to identify potential bioprivilged molecules, that is, molecules that are accessible from biological feedstocks and processes and serve as candidates for conversion to a full range of attractive products via selective chemical catalytic chemistries. Intriguingly, the ranking of potential bioprivilged molecules relies on unfurling potential reaction pathways from the candidate molecule to products of interest and calls for quantitative comparisons of kinetics, which demonstrates the confluence of kinetic modeling and data science and their symbiotic relationship.

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Linda Broadbelt is Sarah Rebecca Roland Professor in the Department of Chemical and Biological Engineering and the Associate Dean for Research of the McCormick School of Engineering and Applied Science at Northwestern University. She was Chair of the Department of Chemical and Biological Engineering from 2009-2017. She was also appointed the Donald and June Brewer Junior Professor from 1994-1996. She has completed the short course Business for Scientists and Engineers through the Kellogg Graduate School of Management. Her research and teaching interests are in the areas of multiscale modeling, complex kinetics modeling, environmental catalysis, novel biochemical pathways, and polymerization/dem polymerization kinetics. She served as the Past Chair, Chair, First Vice Chair and Second Vice Chair of the Catalysis and Reaction Engineering Division of AIChE, and also previously served on the Executive Board of the National Program Committee of AIChE. She is currently an Associate Editor for Industrial & Engineering Chemistry Research. Her honors include selection as the winner of the R.H. Wilhelm Award in Chemical Reaction Engineering from AIChE, the E.V. Murphree Award in Industrial Chemistry and Engineering from the American Chemical Society, the Dorothy Ann and Clarence Ver Steeg Award, a CAREER Award from the National Science Foundation, and an AIChE Women’s Initiative Committee Mentorship Excellence Award, selection as a Fellow of the American Association for the Advancement of Science, a Fellow of AIChE, and a Fulbright Distinguished Scholar, appointment to the Defense Science Study Group of the Institute for Defense Analyses, and selection as the Su Distinguished Lecturer at University of Rochester, Ernest W. Thiele Lecturer at the University of Notre Dame and the Allan P. Colburn Lecturer at the University of Delaware.