The CATALYSIS SOCIETY of Metropolitan New York
www.nycsweb.org

Chair
Jihad Dakka
Jdakka48@gmail.com

Treasurer
John Brody
John.F.Brody@Exxonmobil.com

Student Representative
Samuel Moore
scmoore@princeton.edu

Thursday, April 18th, 2024, 5:30PM
222 Bowen Hall
70 Prospect Avenue, Princeton, NJ, 08540

Prof. Jesse Bond

Biomedical & Chemical Engineering
Syracuse University

Modelling and analysis of transient phenomena in catalytic flow reactors

Packed bed reactors are workhorses in the measurement of reaction rates over powdered catalysts. They are straightforward and inexpensive; one can (usually) operate them under conditions of kinetic control; and one can easily vary their operating conditions to sample the dependence of reaction rates on temperature, pressure, and composition. Moreover, by operating packed beds differentially, they can be approximated as having uniform temperature, pressure, and composition, which avoids spatial integration of material balances and allows one to calculate reaction rates directly from effluent flowrates. As such, packed beds are indispensable for obtaining the macroscopic observables—turnover frequencies, apparent barriers, and apparent reaction orders—that can reconcile with predictions from a microkinetic model.

Experimentalists tend to view flow reactors through a steady-state lens. This makes for straightforward mathematical analysis, but it can be remarkably difficult to define the “steady” state of the catalyst. Multiple concurrent (and coupled) dynamic phenomena impact both the state of the

catalyst and the measurements that we make at the reactor exit. For example, all flow reactors have a hydrodynamic residence time that dictates the rate at which the reactor volume is exchanged. In addition, surface coverages (and thus reaction rates) reach steady state on time scales commensurate with turnover frequencies. Depending on the system, these intrinsic dynamics may be fast, or they may persist for hours. In the latter cases, natural transients in surface coverage often convolute with slow deactivation, induction, or restructuring, and it becomes impossible to confidently define a turnover frequency.

At a minimum, modelling transient phenomena in flow reactors can help to resolve intrinsic kinetics in cases where the state of the reactor and/or the catalyst is changing as a function of time. More significantly, transient responses in catalytic flow reactors are data rich. By developing robust tools for the temporal analysis of flow reactors, we can fully leverage the deliberate introduction of transient phenomena—such as in a SSITKA experiment—to reveal distinct time scales for elementary processes and improve confidence in our estimation of kinetic parameters. Here, we discuss dynamic phenomena in catalytic reactors, and we consider the analysis of data obtained away from steady state. We resolve the implications of catalyst deactivation in differential and non-differential packed beds, and we provide rigorous quantification of turnover frequencies in such systems. Further, we discuss the analysis of inherently transient methods, such as SSITKA.

Speaker Bio

Jesse Bond received his B.S. in Chemical Engineering from Louisiana State University, where he developed an interest in catalysis and reaction engineering. His PhD and Postdoctoral training were under the guidance of Thatcher Root and Jim Dumesic in the Department of Chemical and Biological Engineering at the University of Wisconsin, Madison. He is presently a Professor in the Department of Biomedical and Chemical Engineering at Syracuse University. His research group focuses on developing and understanding catalytic technologies for upgrading abundant natural resources.

Schedule TBA

Student Presentation	5:30 PM
Social Hour (Cash Bar)	6:00 PM
Dinner	6:45 PM
Presentation	7:30 PM

Meeting Fees

Professional Members	$40
Non-members	$50
Students	$25 (Student Members = $10)
Retired/Post-Doc/Unemp.	$40 (Members = $30)
Annual Membership Dues	***$35 (Students = $15)***

Deadline for reservations is **5:00PM Monday, April 15th, 2024**

Please RSVP online using the online form.

To renew your membership, please visit this link.