

5th Annual AIChE Midwest Regional Conference

January 31st – February 1st, 2013

Organized by the Chicago Local Section of the AIChE

Hosted by the Illinois Institute of Technology, Chicago, IL

Session Th1C: 10:00am -11:30am, Thursday January 31, 2013 (Trustee Room)

New, Sustainable Routes to Chemicals and Fuels

Session Organizer: Justin Notestein, Northwestern University

Session Chair: Justin Notestein, Northwestern University

10:00am Steady-Flux Regulation at Primary Metabolic Nodes and Design Implications for Products

Karthik Sekar and Keith Tyo, Northwestern University

Understanding how cells regulate flux in response to heterologous pathways allows engineers to maximize conversion and productivity toward desired products. We characterize flux regulation with respect to native pathways and a heterologous pathway to poly-3-hydroxybutyrate (PHB) in *Escherichia coli*. We find that glucose uptake can be increased from wild-type condition to recover NADPH and when oxidative phosphorylation saturates, lactate secretion relieves electron imbalance.

10:20am Quantifying CO₂ Binding on Titania Based Nanocomposites Using Quartz Crystal Microbalance

Kevin C. Schwartzenberg and Kimberly A Gray, Northwestern University

The first step in photocatalytic reduction of CO₂ is the adsorption and activation of CO₂ on the surface of the catalyst. Titania nanomaterial surfaces contain many sites which can differ in titanium coordination number and Lewis acidity or basicity. This heterogeneity can lead to several different species of adsorbed CO₂ including carbonates, bicarbonates, and carboxylates. Co-catalyst materials may also participate in adsorption. Using quartz crystal microbalance (QCM) technique, we quantitatively probe adsorption and reaction under controlled reaction conditions and explore the role of surface site features and co-catalysts on these processes.

10:40am The Shale-to-Well Energy and Environmental Impacts of Shale Gas Production in China

Yuan Chang, Northwestern University, Robert J. Ries, University of Florida, Runze Huang and Eric Masanet, Northwestern University

Tapping its large reserves of unconventional gas, China has launched shale gas exploration and started drilling wells in trial development zones. To completely understand the energy and environmental impacts of shale gas production in China, this study developed a process-based hybrid life cycle inventory (LCI) model for estimating the ‘shale-to-well’ energy and emissions. Results show that the ‘shale-to-well’ energy for constructing a typical shale gas well in China was 55820 GJ, and the share of upstream and on-site energy was 39% and 61% respectively. The on-site energy depends on diesel consumption, and 54% of on-site diesel was used for oil-based drilling fluid. The product chain greenhouse gas (GHG) emissions were 5120 tons carbon dioxide equivalent, and were dominated by the upstream diesel refining and the fugitive methane in well completion. This study represents an approach to completely quantify the energy and environmental impacts of shale gas production in China, identifies opportunities for impacts reduction, and further contributes to the understanding of potential energy and environmental implications of the ‘coal-to-gas’ transition in China.

11:00am Kinetics of Reaction of Fructose to form 5-(hydroxymethyl) furfural

Anirban Das, Jing Zhang and Eric Weitz, Northwestern University

The acid-catalyzed dehydration of fructose is important in the effective utilization of biomass. This reaction can lead to production of 5-hydroxymethyl furfural (HMF) that can be readily converted into other useful molecules, such as dimethylfuran, furan dicarboxylic acid, gamma-valerolactone, and levulinic acid, which, in turn, can be converted to liquid transportation fuels and chemical feedstocks. The design of an efficient catalyst for this process requires knowledge of the details of the reaction mechanism in order to pin-point the steps that limit selectivity and rate. In the current study, the mechanism of acid-catalyzed dehydration of fructose to form HMF was probed by studying the kinetics of this reaction with an Amberlyst 70 catalyst in DMSO. Kinetic data for the different tautomers of fructose were obtained at different temperatures, acidity and catalyst to reactant ratios. The implications of all of the kinetic data with regard to the magnitudes of the rates that are observed for different reaction steps, and the rate limiting step in the reaction, will be discussed. This study of the kinetics of the formation of HMF from fructose, and influence of the rate of reaction of individual tautomers on the overall reaction process, provides data that are inputs to the development of a complete molecular level model of the kinetics of the reaction of fructose. We anticipate that these data can be used to optimize the production of desired products and guide the development of new catalysts for the formation of HMF with high efficiency and selectivity. This material is based upon work supported as part of the Institute for Atom-efficient Chemical Transformations (IACT), an Energy Frontier

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