

CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING

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Our seminar

“DEVELOPING AN ELEMENTARY, UNIVERSAL DESCRIPTION OF KETONE HYDROGENATION KINETICS IN CONDENSED MEDIA”

Our laboratory aims to develop and understand catalytic technologies that allow production of industrial commodities from renewable or unconventional resources. A central focus is transforming abundant carbohydrates into a suite of products that are either identical to or functionally equivalent to conventional, petroleum-derived fuels and chemicals. A core challenge in converting bio-based compounds to petrochemical commodities is that carbohydrates are deeply oxygenated relative to the intended targets. For example, molecules in hydrocarbon fuels contain no oxygen, whereas carbohydrates have an oxygen-to-carbon ratio of 1. This implies the majority of biomass upgrading strategies will be reductive in nature. Specifically, they will be geared either toward decreasing the oxidation state of specific atoms within a given molecule or complete removal of oxygen atoms from a given molecule.

Often, in the course biomass upgrading, one encounters carbonyl compounds. Monomeric sugars inherently contain reducing ends; aldehydes and ketones are commonly found in “bio-oils;” and furan-aldehydes and oxo-carboxylic acids can be prepared by sugar dehydration. Many of the refining strategies we envision for such molecules are therefore, in line with an overarching tendency toward reductive chemistries, based on carbonyl hydrogenation. For example, sugar hydrogenation yields sugar alcohols, which are common sweeteners in sugar-free food products, and furfural hydrogenation delivers furfuryl alcohol, an important component of resins and adhesives. Of specific interest in this presentation is the hydrogenation of levulinic acid (4-oxopentanoic acid) to form γ -valerolactone, which is a popular precursor of various fuels and chemicals.

The core chemistry of levulinic acid hydrogenation is reduction of a ketone moiety via addition of molecular hydrogen. This is a metal-catalyzed reaction, and supported Ru is the most popular choice for this system. Levulinic acid is a polyoxygenate; therefore, it has a low vapor pressure and is relatively reactive. As with many biomass derivatives, levulinic acid is generally processed in the liquid phase using polar solvents, the nature of which can profoundly impact catalyst performance. Unfortunately, the solution phase is thermodynamically non-ideal, and the kinetic effects of solvation are subtle and often difficult to resolve at an elementary level. Compounding this challenge, supported metals are often “poorly-behaved” in condensed media, with solvents often inducing deactivation and restructuring. Finally, carbonyl hydrogenations are facile, requiring that one must ensure rapid diffusion in order to measure reaction kinetics: this is often non-trivial in solution. Considering the subtle influences of solvation and the numerous confounding phenomena facing experimental acquisition of kinetic data in liquid phase reactions, it is not surprising that a clear view of solvation’s role has yet to emerge.

Here, we consider the kinetics of ketone hydrogenation in both gas and solution phases. In doing so, we attempt to quantitatively decouple the confounding effects of deactivation, restructuring, and solvation to extract true hydrogenation rates, which are then reconciled with an elementary description of ketone hydrogenation kinetics through a microkinetic model.

THURSDAY, SEPTEMBER 22, 2016

COOKIES AND COFFEE -- 1:30 P.M.

SEMINAR -- 1:45 P.M.

SARKEYS ENERGY CENTER, M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971

Accommodations on the basis of disability are available by contacting the office.