DEPARTMENT OF CHEMISTRY
Schlaf Research Group
(www.marcelschlaf.com)

SYNTHESIS • ANALYSIS • INSIGHT

Research and Motivation

With an estimated annually sustained abundance of ~ 200 Gt, ligno-cellulose from plants is the only renewable carbon resource available on a large enough scale. Its highly desirable utilization as the main source of liquid fuels and chemicals is however faced with two fundamental challenges:

i) the depolymerization of ligno-cellulose into its C5-xylose (from hemi-cellulose), C6-glucose (from cellulose) and C9-propyl-catechol (from lignin) constituents.

ii) the deoxygenation of these constituents to more to high-value added chemicals.

Challenge i) can be met either by a non-selective "brute-force" pyrolysis approach resulting in the formation of bio syn-gas (CO/H_2 mixture), bio-char and pyrolysis bio-oil, which possibly can be upgraded to a usable fuel using catalysis or by a combination of mechanical and solvation and acid-catalyzed hydrolysis treatments yielding soluble monomeric sugar (derivatives) and phenols according to the principal transformation A-O-B + H_2O –> AOH + HOB. Challenge ii) can be met by an iterative reaction cascade that combines acid-catalyzed dehydrations with metal-catalyzed hydrogenations, which is conceptually summarized in Figure 1.

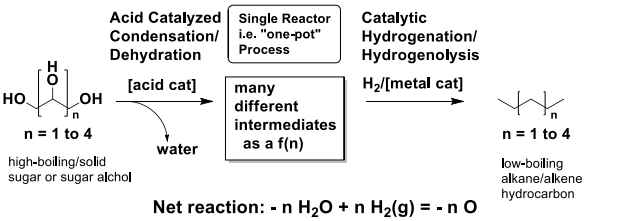

Figure 1: Prinicple Reaction Cascade for the Catalytic Deoxygenation of Carbohydrate Biomass to Hydrocarbon Fuels and Chemicals.

By definition this process requires hydrogenation/hydrogenolysis catalysts that are acid-, water- and high-temperature stable. Using high-pressure reactors and a variety of analytical techniques research in the Schlaf Group focuses on the systematic design, synthesis, testing and development of homo- and heterogeneous catalysts systems that can meet the second challenge.

Current projects target value-chains that emerge from the the hydrodeoxygenation of C5 (xylitol, furfural) and C6 (sorbitol, 5-hydroxymethyl-furfural, 2,5-dimethylfuran) sugar alcohols and condensates to value-added diols, triols, oxacycles (THF's), ethers, alkenes and alkanes using combinations of acid, heterogeneous catalysts and homogeneous catalysts based rationally designed water-stable ruthenium complexes with pyridine-based ligands. Figure 2 illustrates the concept using the extreme case of a total HDO of glucose to hexane as an example with partial deoxygenation, e.g., leading to 1,6-hexanediol as a Nylon precursor being the ultimate goal.

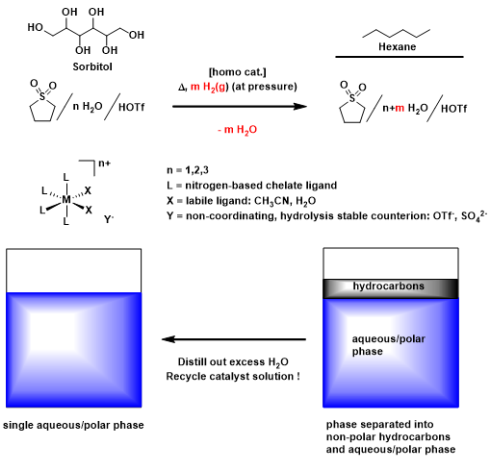

Figure 2: Example of a desired catalytic deoxygenation targeted.

Equipment

The equipment set-up in the Schlaf group goes beyond what is usually found in academic laboratories and more closely resembles what is found in the (petro)-chemical industry. Specifically we use high-pressure reactors for most of our catalytic reactions.
… and yes, you get to use it all by yourself !

Three of our Autoclave Engineers Pressure Reactors with our H_2(g) uptake measurement and data acquisition system.

Equipment in the group's four laboratories:

- Full synthetic lab with Schlenk lines, glassware and glove-box.
- GC, GC-MS/MS, micro-GC (for gas analysis), HPLC-UV/IR.
- CHNS/O elemental analyzer (funded by Rio Tinto ALCAN)
- Karl-Fischer Titroproessor
- 5 benchtop high-pressure hydrogenation reactors
- **CFI funded in 2012 and unique at a Canadian University:** Dedicated 600,000 $ explosion-proof high-pressure hydrogenation lab with three Hastelloy reactors capable of reaching 500 °C at 5,000 psi H_2(g) pressure and real-time gas-flow/temperature/pressure/stirring/sampling control.

Equipment accessible in the department/college/university:

- 300 (multi-nuclear), 400, 500 (solid state), 2× 600 and 800 MHz NMR.
- UV, IR and Raman spectrometers.
- TEM, SEM microscopy and BET analyzer.
- Powder XRD and single crystal X-ray crystallography.
- Hi-Res MS, MALDI-TOF, ICP-MS and AAS, DSC, TGA.
- Excellent machine and electronics shops and glassblower services.
- Excellent electronic resource collection through the UofG library server (SciFinder, Web of Science, Journals, etc.)

Funding & Collaborations

The Schlaf Research Group currently receives(d) operating funding from NSERC, the Ontario Ministry of Agriculture, Food and Rural Affairs (OMAFRA), the US Department of Energy, the Canada-Brazil Network (Kinross Gold) and the CAPES Program of the Brazilian Federal Government) and has collaboration and/or active exchanges with Los Alamos National Laboratory in New Mexico, the Dalian Institute of Chemical Physics (Dalian, China) and universities in Minas Gerais, Brazil.

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