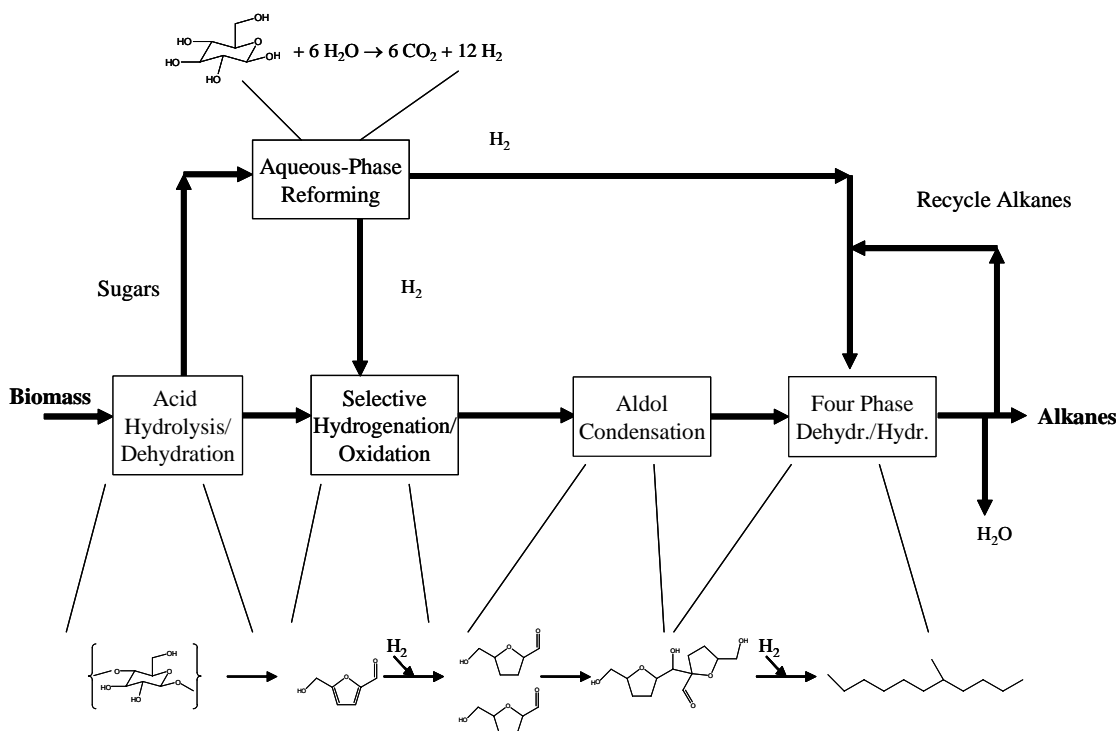


Biorefinery-Sustainable Processing of Alternative Fuels

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Whereas the petrochemical refinery has reached its present state of efficiency by continuous improvement over the past 50 years, the biorefinery is in its infancy. New catalysts and catalytic processes must be developed to provide the flexibility needed for the biorefinery to adjust and optimize its performance to accommodate for changes in feed-stocks and market demands. *The molecular engineering of new catalysts and new catalytic processes for sustainable production of materials and energy from renewable resources requires a vital partnership between educators and researchers in the UC College of Engineering.* The scope of the problem demands a multi-disciplinary, multi-investigator team since the required tools and skill sets, both computational and experimental, span a range not accessible to a single investigator or even a single institution.

Fig. 13. Self-sustaining integrated biorefinery for conversion of biomass into liquid alkanes



Proposed Research:

The development of new catalysts and catalytic processes for the sustainable production of materials and energy from renewable biomass resources will begin at the molecular level. We will:

- employ modern computation methods (e.g., density functional theory) to predict the structures, thermochemical properties, and reactivities of catalytic surfaces that can selectively alter or remove functionality at specific molecular sites of biomass-derived reactants,
- develop synthetic methods to prepare catalysts that exhibit high activity, selectivity, and stability for these biomass conversion reactions,

- utilize advanced spectroscopic techniques to elucidate the atomic-level properties of these catalysts surface under biorenewable conversion reaction conditions.

Moreover, to bridge the gap from these molecular-level studies to the practical development of new processes for biomass conversion, we will:

- employ computational techniques (e.g., dynamic Monte Carlo methods) to predict the dynamics of chemical reactions under practical reaction conditions,
- utilize state-of-the-art simulation tools to address the rates of transport processes under biomass conversion conditions,
- design novel biomimetic reactive separators to achieve efficient conversion of biomass resources into valuable reaction products.
- Search for combining multiple process steps such as acid hydrolysis, hydrogenation and condensation into a single process with development of a multi-functional catalyst.