ABSTRACT

Taufik Ridha Ph.D., Purdue University, October 2018. Transformation of Biomass and Shale Gas Carbon to Fuels and Chemicals. Major Professor: Rakesh Agrawal

In a petroleum-deprived future, sustainably available biomass can serve as a renewable carbon source. Due to its limited availability, however, this biomass resource must be utilized and converted in an efficient manner to minimize carbon losses to undesirable by-products. A modeling and optimization approach that can identify optimal process configurations for chemical and fuel production from biomass using stoichiometric and thermodynamic knowledge of the underlying biomass reaction system is proposed in this dissertation. The modeling and optimization approach consists of two main steps. The first step is generation of the search space and the second step is identification of all optimal reaction routes.

For the first step, literature review and automated reaction network generator, RING, are employed to identify all possible processes for biomass conversion. As these biomass-derived molecules possess multiple functional groups, utilization of automated reaction network generator, which considers a set of biomass-derived molecules and reaction rules, enables generation of all possible reactions. Using this search space, a mathematical optimization problem, which identifies the optimal reaction network, is constructed. The optimization problem identifies all reaction routes with the minimum number of reactions for a given biomass and target molecules. Using this approach, we investigated the following case studies:

1) Upgrading fast-hydropyrolysis vapor of cellulose to higher molecular weight products was investigated. This approach identified a reaction route that can upgrade these molecules to hydrocarbons with carbon number ranging from eight to 12 and this route has not been reported in literature. Preliminary experimental results suggest that the proposed reactions are feasible. This approach has not only revealed unknown reaction routes, but also provided insights for experimentalists for analyzing complex systems.

2) Reducing carbon losses to char during fast pyrolysis necessitated identification of potential pathways for formation of char precursors. Proposed char precursors were identified using mass spectroscopy. Using our approach, potential pathways leading to their formation was identified and these pathways provided initial insights to the potential driving force for the formation of these char precursors and, ultimately, char.

3) Conceptualizing optimal biorefinery configuration using primary processes from C3Bio along with several existing primary processes was examined. Our approach identified biorefinery configurations with carbon efficiencies from 58-63%. These configurations generate both fuel and commodity chemicals. Therefore, this approach not only indicates the appropriate reaction sequences, but also optimal utilization of carbon in biomass-derived molecules. This dissertation provides an initial roadmap toward sustainable production of fuels and chemicals from lignocellulosic biomass.

Considering that the transition to renewable energy is gradual and shale resource is an abundant fossil resource in US, opportunities to valorize shale gas condensate are explored.

Several major shale basins are located in remote locations and historically non-gas producing regions. Therefore, major shale basins regions are lacking the infrastructure to distribute the extracted gas into the rest of the US and particularly the Gulf Coast region. In this dissertation, catalytic shale gas upgrading processes were synthesized, designed, and simulated using Aspen Plus Simulation. Using Aspen Economic Analyzer, preliminary techno-economic analysis and evaluation of its economic potential were assessed at varying scales in order to assess its impact on United States chemical industry landscape.