Sustainable Bio-Based Chemical Production: Life-Cycle Assessment, Techno-Economic Analysis and Supply Chain Optimization

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The development of sustainable chemical processes from biomass has attracted significant attention as an alternative to fossil-based production. However, designing such systems remains challenging due to multiple sources of uncertainty spanning environmental assessment, biological behavior, process performance, and supply chain dynamics. These challenges are especially important for platform chemicals, which often serve as intermediates across multiple pathways and markets. As a result, small changes in modeling assumptions or data can shift resource allocation and pathway selection, leading to different conclusions in both economic and environmental performance.

This dissertation addresses these challenges through a set of methodological and modeling advances aimed at improving the reliability and interpretability of system-level analysis for biomass-derived platform chemicals. First, the impact of uncertainty in life cycle assessment is examined through a detailed study of methodological choices, including system boundary definition, co-product allocation, and carbon accounting. Using carbon-utilization pathways such as triacetic acid lactone as case studies, the results demonstrate that variations in methodological assumptions can lead to notably different sustainability conclusions, highlighting the need for careful interpretation of LCA results in emerging systems.

Second, uncertainty in biological system representation is addressed through the development of a topology-informed approach for identifying metabolic objectives. By combining flux balance analysis with metabolic pathway analysis and a minimum-cut-based formulation, the proposed method quantifies the coefficient of importance (CoI) of metabolic fluxes and enables the identification of distributed objective functions. Application to a co-culture system of *Clostridium ljungdahlii* and *Clostridium acetobutylicum* shows improved agreement with experimental behavior compared to conventional single-objective formulations.

Third, challenges associated with complex and nonconvex design problems are addressed through a topology-informed derivative-free optimization method. By incorporating topological data analysis into particle swarm optimization, the approach adapts the search strategy based on the structure of the solution landscape, leading to improved robustness in identifying high-quality solutions in challenging optimization problems.

Finally, bio-based isopropanol is studied as a representative platform chemical through a sequence of models that progressively incorporate additional system-level complexity. A process and supply chain design model is first developed to evaluate techno-economic and environmental performance, which incorporates geographic information system (GIS). This is extended to a two-stage stochastic formulation to capture uncertainty in feedstock supply and demand. The model is further expanded to include market interactions through an agent-based framework that captures price formation and resource allocation between competing pathways. Together, these studies demonstrate how system behavior and optimal decisions evolve as additional sources of uncertainty and interaction are introduced.

Overall, this work highlights the importance of accounting for uncertainty across multiple scales in the design and evaluation of biomass-derived chemical systems.. The methods and insights developed in this dissertation provide a foundation for more reliable system-level modeling and decision-making in sustainable chemical process design