Process Intensification of Chemical Systems Towards a Sustainable Future

Zewei Chen Ph.D., Purdue University, July 2022. Major Professor: Rakesh Agrawal.

Cutting greenhouse gas emissions to as close to zero as possible, or "net-zero", may be the biggest sustainability goal to be achieved in the next 30 years. While chemical engineering evolved against the backdrop of an abundant supply of fossil resources for chemical production and energy, renewable energy resources such as solar and wind will find more usage in the future. This thesis work develops new concepts, methods and algorithms to identify and synthesize process schemes to address multiple aspects towards sustainable chemical and energy systems.

Shale gas can serve as both energy resource and chemical feedstock for the transition period towards a sustainable economy, and has the potential to be a carbon source for the long term. The past two decades have seen increasing natural gas flaring and venting due to the lack of transforming or transportation infrastructure in emerging shale gas producing regions. To reduce carbon emission and wastage of shale resources, an innovative process hierarchy is identified for the valorization of natural gas liquids from shale gas at medium to small scale near the wellhead. This paradigm shift fundamentally changes the sequencing of various separation and reaction steps and results in dramatically simplified and intensified process flowsheets. The resulting processes could achieve over 20% lower capital with a higher recovery of products.

Historically, heat energy is supplied to chemical plants by burning fossil resources. However, in future, with the emphasis on greenhouse gas reduction, renewable energy resources will find more usage. Renewable electricity from photovoltaic and wind has now become competitive with the electricity from fossil resources. Therefore, a major challenge for chemical engineering processes is how to use renewable electricity efficiently within a chemical plant and eliminate any carbon dioxide release from chemical plants. We introduce several decarbonization flowsheets for the process to first convert natural gas liquids (NGLs) to mainly ethylene in an energy intensive dehydrogenation reactor and subsequent conversion of ethylene into value-added and easy-to-transport liquid fuels.

Molecular separations are needed across many types of industries, including oil and gas, food, pharmaceutical, and chemical industries. In a chemical plant, 40%–60% of energy and capital cost is tied to separation processes. For widespread use of membrane-based processes for high recovery and purity products from gaseous and liquid mixtures on an industrial scale, availability of models that allow the use of membrane cascades at their optimal operating modes is desirable towards sustainable separation systems. This will also enable proper comparison of membrane performance vis-a-vis other competing separation technologies. However, such a model for multicomponent fluid separation has been missing from the literature. We have developed an MINLP global optimization algorithm that guarantees the identification of minimum power consumption of multicomponent membrane cascades. The proposed optimization algorithm is implemented in GAMS and is demonstrated to have the capability to solve up to 4-component and 5-stage membrane cascades via BARON solver, which is significantly more advantageous than the state-of-the-art processes. The model is currently being further developed to include optimization of total cost including capital. Such a model holds the promise to be useful for the development in implementation of energy-efficient separation plants with least carbon footprint. This thesis work also addresses important topics in separation including dividing wall columns and water desalination.