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A Systematic Method for Chemical and Biochemical Sustainable Process Synthesis, Design and Intensification

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In this highly competitive world of chemicals, challenges like ever-increasing energy and utility cost, pressure to increase resource efficiency and new environmental regulations^[1] requires systematic process synthesis-design solutions. The objective of systematic process synthesis-design is to identify the processing route, which gives a desired product from a specific set of raw materials including unit operations design, utility needs, waste generation and sustainability parameters. However, to find innovative and more sustainable process design solutions, extension of the current methods is necessary that can be generated by process intensification. Process Intensification (PI) provides a pathway to design new and innovative solutions or retrofit of existing ones leading to economic, sustainable and efficient solutions. Thus, it is logical to integrate process synthesis-design and intensification to generate more innovative, sustainable and efficient chemical and biochemical solutions.

In this work, a generic three-stage hierarchical decomposition method based on unit operation, task and phenomenon level is applied for sustainable production of succinic acid. This approach examines several succinic acid processing routes from different feeds including bio (glucose, glycerol etc.) and petro (maleic anhydride) based raw materials that are collected through available data and current technologies reported in literature. Using this information, a generic superstructure of processing routes is created that describes a network of configurations representing multiple designs for the production of succinic acid. The next step is to solve the superstructure in order to find the optimal processing route or flowsheet. This has been done through Super-O^[2], a software interface that guides the formulation and optimization of the superstructure to find optimal processing route. Thus, in stage 1, process synthesis is performed to generate an optimal flowsheet among numerous alternatives for succinic acid. In stage 2, the base-case design is developed based on the route selected in stage 1, which is then further analyzed to identify the process hotspots. This is done by first performing simulation to obtain the steady state mass and energy balance data for the selected route. These data are then used for economic analysis, sustainability evaluation^[3] and life cycle assessment^[4] where a set of calculated indicators are used to identify the bottlenecks or process hotspots. These hotspots are then translated to design targets that are used in the next (3rd) stage where, a phenomenon based synthesis-intensification method is applied^[5]. Here, the phenomena are identified by using the PI knowledge base that are representing the tasks performed by unit operations within the base case design. These phenomena are further analysed and re-combined using combination rules to generate new and/or existing unit operations including hybrid operations which in turn are combined to form new and innovative process alternatives. Finally, from the set of feasible intensified process alternatives for production of succinic acid, the best in terms of economic and environmental sustainability is identified.

In this presentation, the implementation of 3-stage method into an integrated multi-scale computer-aided framework will be presented and highlighted by its application to the production of succinic acid to generate more sustainable solutions. The presentation will also discuss the computer aided tools used in this work to achieve the sustainable production of succinic acid.

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