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Integrated & Computer-Aided Product & Process Design: Liquid-Liquid Extraction of Industrially Relevant Organic Acids in biomanufacturing

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Separation and purification processes are responsible for a large portion of the production cost in the bio-processing industry (McGlaughlin, 2012). As such, significant interest and efforts have been geared toward improving existing processes or developing new and innovative ones. Extractive recovery of products from fermentation broth provides an attractive way of separating heat-sensitive or high-boiling products, or products that form azeotropes with water (Kertes and King, 1986). The selective removal of the product using in-situ operation could potentially result in kinetic enhancement of the reaction yielding the desired product. The choice of solvent is a key element in ensuring the extraction process's thermodynamic feasibility and economic viability.

In this work, we present an integrated product-process design framework that combines computer-aided molecular design (CAMD) with a short-cut method for evaluating key process parameters such as product recovery and selectivity. The framework enables the generation of new molecules with desired properties as well as the evaluation of already existing compounds for specific applications. The framework provides a decision-making tool for a more informed detailed simulation and experiments by limiting the chemical design space of viable candidates. This is done by evaluating the pure component properties as well as the mixture properties, both of which are done through quantitative structure-property relations (QSPRs). QSPRs are predictive models that use a numerical translation of the molecular structure and correlate it to the property of interest.

The framework is applied to identify solvents that can selectively extract succinic acid from an aqueous solution also containing acetic acid. The problem is decomposed to first investigate compounds that can:

- Extract succinic acid from an aqueous solution
- Extract acetic acid from an aqueous solution
- Selective extraction of succinic acid from a solution of water and acetic acid

The work will aim to investigate whether currently used thermodynamic and property models are capable of such a task and compare the obtained results to studies readily available in the literature.

References

Kertes, A.S., King, C.J., 1986. Extraction chemistry of fermentation product carboxylic acids. Biotechnol Bioeng 28, 269–282.

McGlaughlin, M.S., 2012. An Emerging Answer to the Downstream Bottleneck. Bio-Process International 10 (5) 58–61.

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