

## Physical Property Data and Models in Support of Bioprocessing Separation Technologies for Organic Acids Separation

We propose to collect physical property and thermodynamics data for impactful bio-products and their separations, to build thermodynamic models to represent the behavior of multi-component mixtures, and to incorporate these models into process simulation environments to allow for faster and cost-effective scale-up of bio-separations technologies. The proposed work specifically targets the separation of organic acids from multicomponent mixtures typically encountered in bioprocess operations, using three distinct separation technologies: adsorption, membranes, and electrochemical techniques.

This proposal forms an alliance of academia-industry-national lab to develop a methodology for modeling the full process of bio-separation units for both single and multi-component systems. The proposed methodology will include the collection and incorporation of physical property data to thermodynamic models, and their connection to commercial process simulation environments supporting the scale-up and development of membrane, electrochemical, and adsorption-based processes for separation and recovery of organic acids from aqueous solutions (e.g., fermentation broth, lignin-rich streams, etc.) as well as vapor phase bioproducts (e.g. isoprenol). The consortium will develop a methodology to model the full process of bio-separation units for both single and multi-component systems. By bringing together a combination of experimental and modeling expertise, the proposal entails to facilitate the scale up predictions and design of key bioseparation technologies. The project team will leverage on experimental data generation to build thermodynamic models that will be input into bioseparation process models along with the relevant kinetic parameters. The process models will be compared and verified to scale up separations processes for pilot experiments. With guidance from the simulation software partners, the project team will perform the implementation and application of the data and models in commercial process simulators. The development of advanced Machine Learning based models to speed up the simulation performance will also be incorporated.

The project work will be led from the RAPID Manufacturing Institute, a dba of the American Institute of American Engineers by Dr. Ignasi Palou-Rivera as PI. RAPID will coordinate the project work, perform Project Management duties, participate in process model and flowsheets development, lead TEA, LCA and Tech-2-Market tasks, and coordinate the Industry Board. Argonne National Lab will lead the experimental work both at bench and pilot scales. Texas Tech University will be the key partner in thermodynamic and basic process modeling. Siemens Technology will lead the Machine Learning Activities. Siemens PSE will actively work on process modeling and incorporate advanced unit modeling to its flagship commercial simulator gPROMS, as well as contribute licenses and participate in the Industry Board. The other two commercial simulator companies, AspenTech and Chemstations, will contribute to the project by providing licenses to their software and participate in the Industry Board. Representatives of DIPPR, and potentially of other data and standards organization such as NIST, will also be connected to the project work through the Industry Board advisory role.