Modeling and Simulation

Vision

Through the development of enabling methods, tools and open-source software that employ a multi-scale, integrated, and systems-level approach to process intensification design, optimization, and control, this focus area will address the challenges inherent to:

- Modular process intensification of periodic separation processes (e.g., pressure swing adsorption, vacuum swing adsorption, temperature swing adsorption, simulated moving bed)
- Process intensification of micro-reactor and heat exchange processes (e.g., micro-reactors for stranded natural gas conversion)
- Modular process intensification via process integration of existing processes.

Objectives

- Intensification of adsorption-based modular separation processes with periodic operations to reduce emissions from diverse sources and utilize many unconventional feedstocks.
- Parallel development of complimentary reaction and separation modules that will effectively integrate into a stable, safe, and economical modular chemical process.
- Multi-scale toolset for the rapid identification, design and refinement of modular chemical transformation and chemical separation technologies for process intensification via modularized units.
- Development of methods, tools, and open-source software for design, optimization, and intensification across multiple length and time scales.

Key Approaches

- Multi-scale representation, modeling, and optimization for process intensification.
- Integrated materials design and process optimization.
- Optimization tools for models under uncertainty.
- Robust and decentralized control strategies and tools.
- Incorporation of operability and safety criteria in modeling, optimization, and control.

Expected Outcomes

- Device- and process-scale tools necessary for rapid module design and development, with the ultimate goal of generating open source software and publicly-disseminated design rubrics for the enhancement of the scientific and industrial community.
- A new design paradigm and the associated computational tools necessary for its efficient implementation, for rapidly identifying cost-effective / energy-efficient operable modular chemical processes
- A set of integration strategies and solutions that span the multiple scales associated with manufacturing.

Contacts

David Sholl, Ph.D.
Lead - Modeling and Simulation Focus Area
Georgia Institute of Technology

Phone: 404-894-2822
Email: david.sholl@chbe.gatech.edu

Stratos Pistikopoulos, Ph.D.
Co-Lead - Modeling and Simulation Focus Area
Texas A&M Energy Institute

Phone: 979-458-0259
Email: stratos@tamu.edu

RAPID's focal point for modeling and simulation efforts within all focus areas