Sustainable Separations for Modular Chemical Manufacturing

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Critical Innovation Challenge

- Distillation consumes ~10% of U.S. energy (6.9 – 8.5 quad).[1]
  - The business of chemistry supports 26% of U.S. GDP and 96% of manufactured goods.[2]
  - Central to chemical manufacturing, fluid separations require >50% of chemical plant investment.[3]
  - Reliance on distillation accounts for >40% energy use in the CPI.[4]
  - Technology infrastructure is optimized for distillation.
- Mass separating agent (MSA) based processes can make these separations 10X more energy efficient.[1]
  - State of the art in the design of MSAs requires iterative trial & error that takes years to match a mixture with an MSA process to achieve a given separation task.

1 Sholl and Lively, 2016. Seven separations to change the world, *Nature*.
2 ACC, 2016. The Business of Chemistry: By the Numbers.
3 King, 1980. *Separation Processes*, 2nd edition.
4 Humphrey and Keller, 1997. *Separation Process Technology.*

ALTSEP Overview

Group: Innovators from the chemicals sector, technology suppliers, universities, and government.

Aim: Transform the separations technology infrastructure to accelerate industry-wide application of energy-efficient alternative separation (ALTSEP) processes where they can be more sustainable than distillation.

Approach:

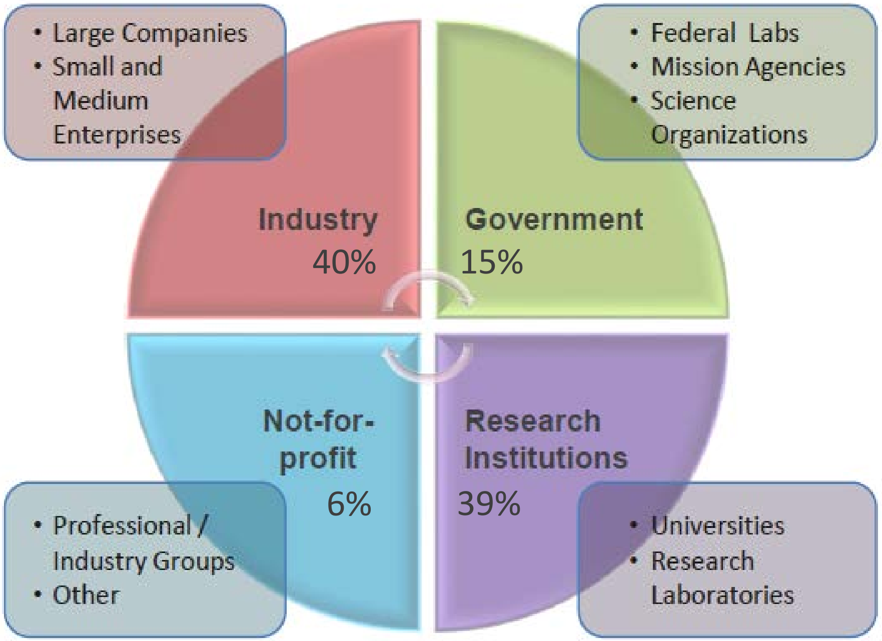
- Create a roadmap to identify and prioritize RD&D projects needed for predictable industrial application.
- Enable a molecular property-based system for process selection, simulation, and design.
- Catalyze a robust ecosystem across the chemical enterprise to foster industry-wide implementation.

Roadmap sponsored by

Broad Collaboration Base

Albemarle, Arizona Chemical, Chemours, Dixie Chemical, MilliporeSigma, Solvay, AstraZeneca, Merck, Pfizer, Sanofi, AirLiquide, Compact Membrane Systems, Dow, Eastman, Evonik, ExxonMobil, Ingevity, Kroungold Analytical, Membrane Technology & Research, Molecular Knowledge Systems, Novasep, WasteHub

ACS Green Chemistry Institute, AIChE (including IfS, Separations Division, CoMSEF), Industrial Fluid Properties Simulation Collective, Pine Chemicals Association



NIST AMTech, NIST Material Measurement Laboratory, NSF CBET, EPA Office of Research & Development, ORNL, NETL

Auburn, Georgia Tech, Harvard, Imperial College, New Jersey Institute of Technology, Northwestern University, Rowan University, Technical University of Denmark, Technical University of Dortmund, Texas Tech, University at Buffalo, University of California, University of Colorado, University of Delaware, University of Florida, University of Minnesota, University of Notre Dame, University of South Carolina, University of Toledo, University of Virginia

Key Research Areas

- Broadly available, demonstrated, cost-effective MSAs (e.g., adsorbents, membranes) for industrially relevant separations

- Robust models and tools to select, simulate, and design optimal MSA-based separation processes

Reliable, Cost-Effective MSAs

- Molecular simulation and experimental characterization of MSA materials & MSAs in fluids
  - Molecular understanding of material compatibility
  - Discovery of soft disordered materials as effective MSAs
  - Ability to control defects & properties in MSA synthesis
  - Validated property databanks for engineering models
- Rational design of MSA for a separation task
- Screening tools to predict MSA process performance
- Experimental validation predicted performance
- Manufacturability of scalable, sustainable MSAs

Robust Models and Tools

- Mechanistic understanding for reliable prediction of long-term solid MSA process performance (fouling, aging)
- Molecular property-based models of non-ideal, multicomponent sorption and transport in microporous materials and polymers
- High fidelity simulation of solid MSA-based processes compatible with accepted software standards
- Algorithm(s) for synthesis and optimal design of solid MSA and hybrid multicomponent separation processes
- Effective heuristics to identify MSA candidates to consider as options for achieving a separation task

Moving Ahead

- Align research with manufacturing goals
  - Reduce time to market
  - Increase capital productivity
  - Disrupt process energy intensity
- Maintain consistent, sustained research focus
  - Explore integration of reactions and separations
  - Continue development of transferrable force fields (TraPPE) to enable molecular modeling advances
- Promote research coordination