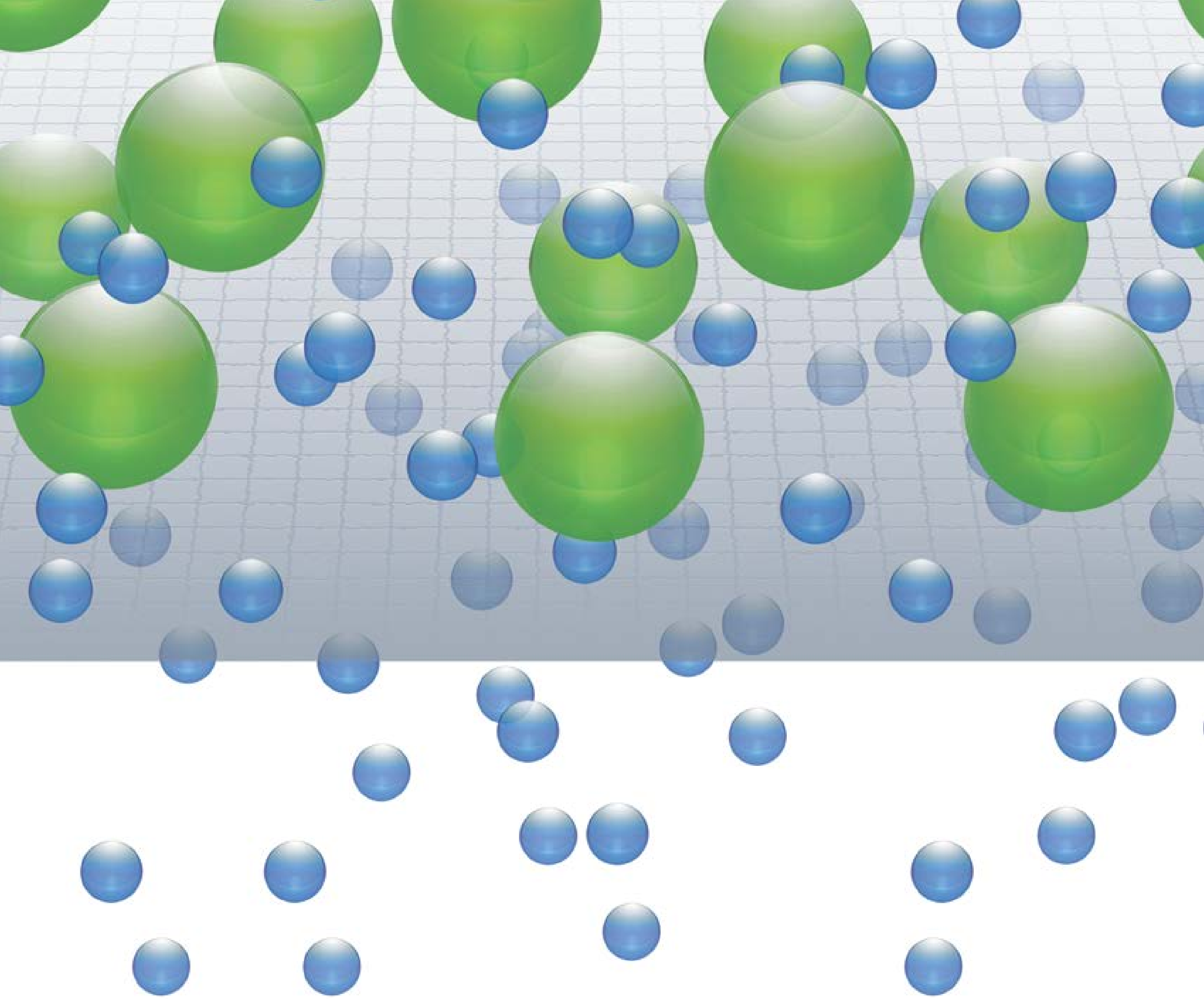

Sustainable Separation Processes

A Road Map to Accelerate Industrial Application of Less Energy-Intensive Alternative Separations (AltSep)

AltSep

ACS Green Chemistry Institute
Chemical Manufacturers Roundtable

NIST National Institute of Standards and Technology
U.S. Department of Commerce

AIChE
The Global Home of Chemical Engineers

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altsep.org

www.acs.org/content/acs/en/greenchemistry/industry-roundtables/chemical-manufacturers.html

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EXECUTIVE SUMMARY

The chemical industry is composed of many diverse manufacturers making products essential and desirable for society and the economy. Chemical manufacturing processes consume large amounts of energy, and one feature shared by virtually every chemical manufacturing facility is the separation process. The most common process to separate mixtures in the chemical processing industries (CPI) is distillation. The installed base of thousands of highly functional distillation columns across industry supports today's separation needs. Although the overall savings and sustainability gains afforded by less energy-intensive alternatives would be significant, distillation's strong incumbency advantage, combined with a significant but finite number of technical barriers associated with alternatives to distillation, has hindered investigations into lower-energy industrial separation processes. The required changes are so fundamental and significant that they are beyond the reach of any one company to achieve in isolation.

The goal of the AMTech planning project was to create a technical innovation road map for advancing the rational design and predictable, widespread, industrial application of less energy-intensive separation processes as alternatives to distillation. Instead of continuing to rely on thermally (or pressure) driven separation processes based solely on relative volatility (distillation), this project took a cross-cutting, integrated, translational approach to identifying and prioritizing the research, development, and demonstration (RD&D) needed to solve technical challenges starting at the molecular level. This road map is intended to stimulate the exploration of molecular property-driven (e.g., molecular volume, molecular shape, dipole moment and polarizability, molecular charge, and chemical reactivity) alternatives that are more effective and energy-efficient separations technologies.

The AltSep Road Map outlines nine key RD&D needs, as seen in the table on pages 5–7. For more detailed information, please see Section 5 of this report.

Now that the most promising molecular property-focused RD&D projects are identified, technology solutions may be further researched and developed until sufficient technology demonstrations have been completed and adequate process simulation tools have been developed. Precompetitive collaboration among innovators from chemical (including pharmaceutical) manufacturers, universities, professional organizations, and research institutions is essential to move this initiative forward. The ultimate goal of the AltSep initiative is to catalyze the creation of a robust ecosystem across the chemistry enterprise to foster RD&D projects that lead to widespread industrial implementation of less energy-intensive alternative separations technologies.

Key Research, Development, and Demonstration Needs

1. Develop organizational and technological infrastructure to expand and accelerate Mass Separating Agent (MSA) research, development, and demonstration (RD&D).

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Create a center of excellence in alternative separations RD&D.	🟩	🟩	
Enable widely-available high-performance computing through advances in computer architecture and cost-effective access.		🟩	🟩
Develop educational resources to equip students to solve high-mass flux separations starting at the molecular level.		🟩	🟩
Develop MSA-based unit operation case studies for educational purposes (i.e., workforce development, textbook chapter, AIChE short course, teaching lab in senior design, Master's program).		🟩	🟩

2. Identify intrinsic molecular properties, descriptors, and interactions, beyond those used for distillation, to direct exploration.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Implement analytical separations techniques that use different molecular and physical properties for separations.			🟩
Develop molecular topology descriptors and novel experimental techniques to measure intermolecular interactions.	🟩		
Perform experimental studies on the effect of fluid and MSA on intermolecular interactions at varying distances from interfaces.	🟩	🟩	
Develop molecular-level understanding of material/fluid compatibility.		🟩	🟩

3. Establish theoretical underpinnings of molecular property-based design of separation alternatives.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Formulation of new theories for nondilute liquid thermodynamic and transport behavior in membranes		🟩	🟩
Experimental/computational studies to lead to robust theory capable of predicting multicomponent adsorption equilibria from single component isotherms	🟩	🟩	🟩
Formulation of external field separation theories and models		🟩	🟩
Theoretical understanding of aging and fouling mechanisms		🟩	
Develop fundamental molecular-level understanding of MSA materials and materials compatibility.		🟩	🟩

4. Develop infrastructure for data warehousing and open access to support molecular property-driven alternative separation technology RD&D.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Agree on ontology and standards for characterization, interaction, transport, and interface data and make available in curated repositories.	🟩	🟩	
Develop, validate, and curate molecular, physical, and fluid property databases for use in the development of theory, and in the implementation of modeling and simulation across length and time scales.	🟩	🟩	

5. Develop capacity for modeling and simulation of molecular, physical, fluid and bulk properties and interactions (inter- and intramolecular, at interfaces, n-body, MSA-fluid) across length and time scales.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Develop effective heuristics to identify MSA candidates to consider as options for achieving a separation task.	🟩		
Develop molecular property-based models of non-ideal, multicomponent sorption and transport in microporous materials and polymers.		🟩	🟩
Perform systematic coarse-graining of interactions in highly complex mixtures (>1,000 components) to adapt individual species forcefields into lumped models.	🟩	🟩	
Develop multiscale separation process models that cover the range from molecular property prediction to continuum models for computer-aided scale-up.		🟩	🟩
Develop flow models for industrial scale membrane modules to relate fluid distribution and properties to performance.		🟩	🟩
Perform high-fidelity simulations of MSA-based processes (w/ or w/o fields) that are compatible with standardized, accepted, and validated software standards.	🟩	🟩	
Develop algorithm(s) for synthesis/optimal design of MSA and hybrid multicomponent separation process sequences.	🟩	🟩	
Develop cost estimation tools to enable MSA selection and process optimization.	🟩	🟩	
Develop screening tools to predict MSA performance in a proposed process.	🟩	🟩	
Develop sustainability assessment tools to profile the impacts of different MSA and associated unit operations.	🟩	🟩	

6. Discover and develop novel, well-characterized, and well-understood MSA materials (i.e., adsorbents, membranes).

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Discover novel MSA materials and MSA synthesis techniques to ensure effective, reproducible, and robust MSA performance.		🟩	🟩
Perform computational/experimental studies to relate thermodynamics and dynamics of solute–surface interactions to MSA selectivity.	🟩	🟩	
Develop fundamental quantitative understanding of MSA surface and structure that enables rational design, e.g., develop novel instrumental techniques, etc. *(see Section 5 for more information)*.	🟩	🟩	
Develop experimental methods and studies to determine effects of adsorbed molecules (e.g., contaminants, nontarget molecules) on MSA structure, transport properties, robustness, and aging.	🟩	🟩	
Develop high-throughput testing capacity and novel analytical techniques to systematically measure and characterize bulk MSA-molecule-fluid-intermolecular interactions and separation behavior.	🟩	🟩	
Develop fundamental understanding of the effect of fluid and MSA on intermolecular interactions at varying distances from interfaces.		🟩	🟩
Determine the impact of pellet/film/fiber forming on molecular transport.	🟩	🟩	
Determine the effects of adsorbed molecules (e.g., contaminants, nontarget molecules) on MSA structure, transport properties, robustness, and aging.	🟩	🟩	
Develop fundamental understanding of organic-salt-particle-water interactions in solid/liquid separations for pretreatment.		🟩	🟩

7. Develop understanding of the influence/effect of external fields (e.g., electric, magnetic) on MSA-based separations.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Design and synthesize functionalized, field-switchable particles and meta-materials.		🟩	🟩
Investigate external field effects on fluid structure, energetics, and transport properties to assess feasibility.	🟩	🟩	
Discover stimuli-responsive, field-tunable MSA materials for separation and fouling prevention.		🟩	🟩
Develop electromagnetic materials for field source.		🟩	🟩
Develop applied field-enhanced MSA modules (e.g., source within module).			🟩
Develop standards for applied fields and field uniformity.	🟩		
Develop novel technologies for low-energy elution and desorption.		🟩	🟩

8. Develop favorable, predictable, robust, and stable, high-performance process configurations.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Investigate, evaluate, develop, and demonstrate hybrid separation processes and benchmark systems, separative reactors, etc.	🟩		

9. Develop capacity for predictable, reproducible, robust, and stable process performance and demonstrated performance and manufacturability of scalable, sustainable MSAs and MSA-based processes.

STEP	SHORT-TERM	MEDIUM-TERM	LONG-TERM
Develop advanced sensors for in situ diagnostics and real-time control.		🟩	🟩
Develop flow models for industrial-scale membrane modules that relate fluid distribution and properties to performance.	🟩	🟩	
Develop models for unit operations and operation mechanicals.	🟩	🟩	
Discover and pursue mechanistic understanding of membrane fouling mechanisms (physical, chemical, biological) across a wide range of real-world, complex, liquid separation tasks.		🟩	🟩
Facility(ies) for long-term, commercial-scale demonstration, with standard protocol for facile module connection			🟩
Standardized module fabrication platform and facility(ies) for producing pilot-scale modules			🟩

1. Technical Challenges with National Impacts

Chemical manufacturing in America is at a crossroads. The business of chemistry supports nearly a quarter of the nation's gross domestic product.[1] The chemical processing industry (CPI) makes products that are essential to society and to the economy. Although many of these chemical products improve the energy efficiency of many commercially available products in use, the manufacturing processes needed to make them consume large amounts of energy. Chemical processing and petroleum refining are the top two U.S. manufacturing sectors in energy consumption[2] and greenhouse gas (GHG) emissions.[3] Carbon dioxide emissions from the chemicals (including pharmaceuticals) sector alone account for about 4% of the total for the United States.[1] Chemical manufacturers have long recognized their energy intensity and the need to reduce energy consumption, not only because of cost, but also because of the environmental consequences of energy production and use. For example, higher energy efficiency is "an important lever" for GHG reductions.[4] Accordingly, leading chemical manufacturing companies have committed to significant energy use reductions over the years. However, despite substantial reductions since 1990, CPI energy consumed per unit of output has been essentially flat since 2012 and has not yet returned to 2006 performance levels.[5] To further improve competitiveness, chemical manufacturers need to take a closer look at all aspects of their processes to achieve deeper cuts in energy use.

One feature shared by virtually every chemical manufacturing facility is the separation process. The most common process to separate fluid mixtures in the CPI is distillation, which accounts for more than 40% of the energy used in the CPI.[6] This equates to more than 10% of energy use nationally.[7] Therefore, reducing the energy required for the fluid separations at the heart of chemical processes is fundamental to assuring the sustainability and global competitiveness of the U.S.-based chemical enterprise. The more sustainable, more competitive road ahead is the one where less energy-intensive alternatives to distillation are broadly understood and widely practiced in the industry. However, to find their way down that road, the members of the chemical industry need a map.

The goal of this AMTech planning project was to create an innovation road map for advancing the rational design and predictable, widespread, industrial application of less-energy-intensive separation processes as alternatives to distillation. The collaboratively developed road map identifies and prioritizes RD&D technology initiatives with the potential to transform the competitiveness and sustainability of the U.S. chemical enterprise.

1.1 Grand Challenge

To help the nation and the CPI define a path toward a "sustainable chemical enterprise", the National Research Council (NRC) outlined eight grand challenges for addressing sustainability in the CPI in the 21st Century.[8] Prominent among these was the grand challenge of reducing the energy intensity of the chemical and allied process industries. Noting the critical importance of more energy-efficient technology over the period from 2005 to 2025 (while fossil fuels would be the main source of fuel and feedstocks), the NRC called for research to "develop more energy- and cost-efficient chemical separations, especially effective alternatives to distillation".[8] Having the use of distillation and a shared aim to reduce energy consumption during chemical manufacturing in common, the American Chemical Society (ACS) Green Chemistry Institute (GCI) Chemical Manufacturer's Roundtable member companies embarked on a pre-competitive effort in 2013 to investigate less energy-intensive alternative separation technologies that could competitively displace distillation when new or replacement equipment is being specified.[9] The development of the AltSep Road Map has leveraged the work of the ACS GCI Chemical Manufacturer's Roundtable and expanded the collaboration base of this existing consortium. The RD&D projects identified in the road map are intended to respond to the NRC challenge.

1.2 Industry Need

Energy cost and availability define the competitiveness of chemical manufacturing in the United States. Separation by distillation consumes over 8 quads of energy each year,[7] and equipment for separations generally requires 50 to 90% of the investment in large-scale chemical plants.[10] Exploiting differences in volatility through distillation has been the dominant means of separating components in chemical processes for more than a century. Principles for effective design and operation of distillation processes are taught and well understood by industrial chemists and chemical engineers. The installed base of thousands of highly functional distillation columns across the CPI meets today's separation needs. Distillation is a well-understood, reliable, robust, and predictable separation technology.

Although the overall savings and sustainability gains afforded by less energy-intensive alternatives would be significant, distillation's strong incumbency advantage and a significant but finite number of technical barriers need to be overcome to light the way for the widespread adoption of low-energy separation processes in industry. The required changes are so fundamental and significant that it is beyond the reach of any one company acting alone to achieve even a modicum of progress. Pre-competitive collaboration among innovators from chemical (including pharmaceutical) manufacturing industries, universities, professional organizations, research institutions, separating equipment and separating agent suppliers, national labs, and federal agencies is needed to obtain enough understanding of these barriers to lay out a course of research, demonstration, and development projects that would break them down. The collaborative development of a road map to advance the rational design and predictable, widespread industrial application of less energy-intensive separation processes has identified and prioritized RD&D technology initiatives with the potential to transform the competitiveness and sustainability of the U.S. CPI enterprise.

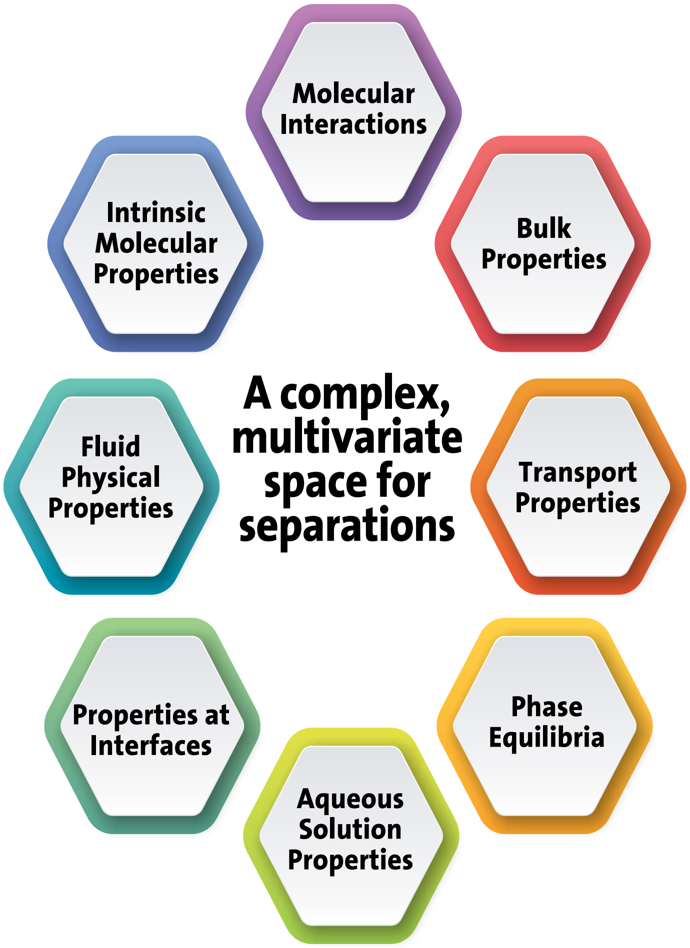
1.3 Scope and Vision

An intrinsic green chemistry approach is consistent with the national strategy for advanced manufacturing.[11] Building on the knowledge and experience of the ACS GCI Chemical Manufacturers Roundtable, and starting at the molecular level, this project took a cross-cutting, integrated, translational approach to identifying and prioritizing the RD&D projects required to solve the technical challenges associated with transitioning to alternative technologies. Although molecular synthesis gets the most attention, the time and effort required to develop efficient and effective isolation and purification processes during the development and commercialization of new chemicals and chemical products is comparable to or greater than that required to develop the synthesis scheme. As a result, discovery and process chemists, together with chemical engineers, are keenly interested in improved separation processes that can be conceived and evaluated based on the intrinsic properties of the molecules to be separated.

Instead of relying on thermally driven (or pressure-driven) separation processes based solely on relative volatility (distillation), AltSep has developed an innovation road map to stimulate the exploration of intrinsic molecular properties (e.g., molecular volume, molecular shape, dipole moment and polarizability, molecular charge, and chemical reactivity)[8] that may be utilized for effective and energy-efficient separations. The emphasis on intrinsic molecular properties (chemistry) made the ACS well-positioned to lead this effort. Understanding fundamental molecular and physical property-based phenomena is an important step toward advancing low-energy separation techniques. Moving beyond reliance on volatility requires innovation across the multivariate space of properties and interactions depicted in Figure 1.

FIGURE 1

Innovation Space for Alternative Separations



1.4 National Outcomes

The availability of predictable, cost-effective, less energy-intensive alternatives to distillation for fluid separations would be a game-changer for chemical manufacturing in the United States for several reasons:

- The potential to significantly reduce the amount of energy currently consumed by distillation would equate to substantial reductions in GHGs and other emissions associated with steam production, electricity generation, and other fuel consumption while bolstering the cost competitiveness of companies in the CPI.
- Having a straightforward molecular properties-based approach to the selection and design of such cost-competitive separation processes would be expected to lead to the recovery of what are now considered only marginally valuable by-products in manufacturing waste streams, thereby further improving the cost competitiveness and environmental performance of the U.S. chemical manufacturing enterprise.
- Achieving the RD&D objectives identified in the innovation road map will lead to the implementation of new technologies, science and engineering tools, and databases in settings such as education, equipment design, and manufacturing, all of which will generate high-technology jobs.
- The energy efficiency improvements associated with alternative separations technologies in combination with the current shale oil and gas cost advantage will lead to enhanced global competitiveness for U.S.-based chemical manufacturing. This enhanced competitiveness is likely to result in further expansion of jobs in the CPI. Every job created in the chemicals sector results in 7.5 jobs generated elsewhere in the American economy.[5]
- The same innovative, transformational technologies stemming from the RD&D outcomes identified in the sustainable separations road map can be deployed in related sectors, such as in bio-based and renewable chemicals production, to effect similar gains to those described above for petroleum-based chemical manufacturing.

1.5 Alignment with Manufacturing USA

The AltSep initiative complements the work of existing Manufacturing USA institutes.

- The Clean Energy Smart Manufacturing Innovation Institute (CESMII) seeks to broadly improve the sustainability and energy efficiency of U.S. manufacturing while increasing industrial competitiveness through the use of advanced sensors and controls. While AltSep has similar goals, and certain projects identified in this road map depend on sensor and control technology, the AltSep initiative is focused on reducing the energy intensity of fluid separation processes common to the chemical process industries through a larger range of process technologies.
- The National Institute for Innovation in Manufacturing Biopharmaceuticals (NIIMBL) is working to enable more efficient biopharmaceuticals manufacturing with a focus on biological technologies for the synthesis of therapeutic drug substances. As with other parts of the chemicals and pharmaceuticals sector, the efficiency and cost-effectiveness of biopharmaceutical commercialization will be enhanced by the implementation of separation technology RD&D projects identified by the AltSep Road Map.
- The Rapid Advancement in Process Intensification Deployment (RAPID) Institute seeks to save energy, reduce waste, and cut operating costs through the intensification of many different chemical processing technologies used in U.S. chemical manufacturing. The AltSep initiative has generally similar objectives, and early AltSep roadmap development efforts were used to help prepare the RAPID proposal and the RAPID Institute Road Map that were submitted to the U.S. Department of Energy. Furthermore, many of the RD&D projects in the AltSep Road Map, especially the ones focused on fundamental research and database development, are as critical to the overall success of RAPID as they are to competitiveness and sustainability progress for the CPI. Implementation of the AltSep roadmap would clearly complement the work of the RAPID Institute.

2. Road Mapping Development

2.1 Project Background

The AltSep project was built on two prior efforts to explore improvements in separation processes. The first[12] developed a separations road map of critical research needs and technical barriers for the advancement of individual separations technologies, and it was created with input from process engineering experts in each field. However, a review of relative energy efficiency, scale, and throughput across the range of separation technologies does not appear to have been a focus. The second[2] ranked major commercial separation processes in terms of energy consumption in chemicals manufacturing (see Figure 2), and it was part of a review of the materials research and development needs of low-energy separation processes (including membranes, adsorption, liquid extraction, and advanced filtration).

After more than a decade, the grand challenge of "energy-efficient separations"[8] remains unfulfilled. The shortfall in widely applicable, commercially feasible, low-energy separation process technology appears to be attributable to two phenomena. First, there is not a critical mass of chemists and chemical engineers focused on translating promising research to commercial reality in the near term. Second, there is not a holistic, integrated approach (i.e., one that balances cost, performance, and sustainability) that is built on fundamental research and a molecular-level understanding of the kinds of separations needed for longer-term improvements in the commercial viability of less energy-intensive alternative separations.

2.2 Separation Process Value Chain

An idealized view of the separation process value chain is shown in Figure 3.

- Funding sources usually include the U.S. Department of Energy and the National Science Foundation.
- Fundamental research on the measurement and prediction of relevant molecular properties generally takes place at universities and in national labs such as the National Institute of Standards and Technology (NIST). Fundamental research in separation process technology is conducted largely at universities, with some conducted at other locations such as Oak Ridge National Labs (ORNL) or specialized contract research facilities.
- There are a variety of actors in the development portion of the separation process value chain, from those engaged in the development of molecular and physical property data and prediction tools, to those developing new separating agents, to firms developing new and improved separations process equipment. The Design Institute for Physical Properties (DIPPR) and NIST are two of the larger developers of molecular and physical property databases relevant to separation process design and operation. Although most separations process equipment development is completed at well-known, larger firms, a meaningful proportion is completed by smaller firms, including those that have been spun off from university research labs.
- The main elements of technology demonstration are confirming operability and scale-up approaches and the formulation of separation process simulation tools for use in the design and optimization of separation processes. Companies specializing in process simulation tools include AspenTech, Chemstations (makers of CHEMCAD), and Process Systems Enterprise (PSE).
- Manufacture and supply depends on the production and fabrication of commercially available separation process equipment and separating agents for sale and distribution to end users. Process equipment companies include Evonik, Filmtec, Koch-Glitsch, W. L. Gore, Pall, and Sulzer Chemtech.
- End users in the CPI include the variety of manufacturing companies across the industry that use one or more separation processes in each of their facilities. Examples of such end users are the member companies of the ACS GCI Industrial Roundtables.

FIGURE 2
Relative Energy Use by Various Separations Technologies

REPRODUCED FROM DOE, 2005

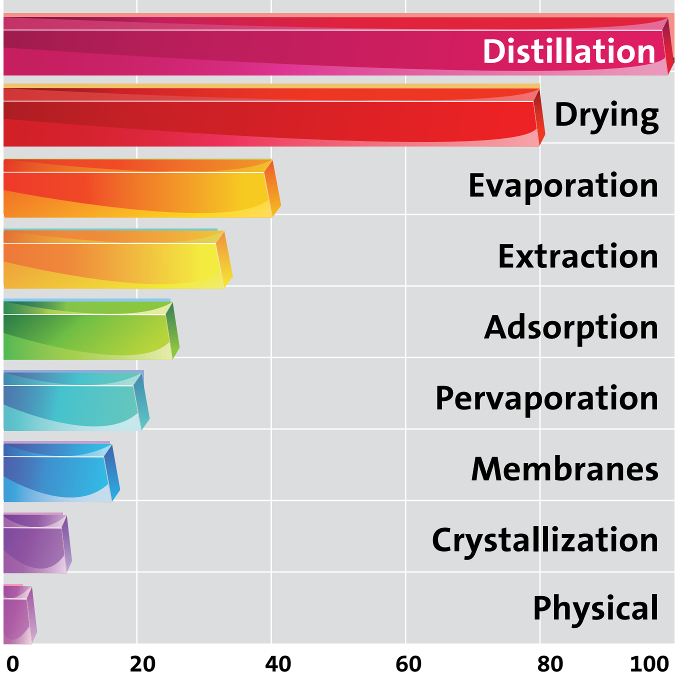


FIGURE 3
Separation Process Value Chain

2.3 Breadth of Participation

The Road Mapping project leveraged the existing consortium of companies in the ACS GCI Industrial Roundtables, principally the ACS GCI Chemical Manufacturer's Roundtable and the ACS GCI Pharmaceutical Roundtable. ACS GCI Chemical Manufacturer's Roundtable member companies most active in the development of this Road Map include: Chemours, Kraton, MilliporeSigma, and Solvay USA, Inc.

Through preliminary outreach efforts, the collaboration base was extended to include NIST, a range of universities, and other national labs doing research in molecular simulation to gain a deeper understanding of the molecular interactions and transport phenomena underlying fluid separation processes. Further outreach brought in several separation process users and a number of separation process technology providers.

2.4 Road Map Development

Road Map development was carried out in phases, as listed below.

Phase 1 — Engage stakeholders

The AltSep team worked to expand the collaboration base beyond the ACS GCI Industrial Roundtables and across the full range of the separation process value chain (depicted in Figure 3); included were separations, physical/chemical property, and other chemical science and engineering innovators from the chemical processing industries, universities, professional organizations, research institutions, separating equipment and separating agent suppliers, national labs, and federal agencies. A hosted website (**www.altsep.org**) promoted stakeholder outreach and facilitated information-sharing throughout the course of Road Map development.

Phase 2 — Develop Road Map

Six workshops were convened; they included experts and other stakeholders identified in Phase 1. Workshop output was used to outline the current state of the art and develop the elements of the Road Map. Workshop participants articulated gaps in fundamental knowledge, the breadth and nature of required data repositories, the degree and nature of standardization, gaps in tools and tool availability, the nature and capability of process simulation programs, mechanisms for best-practice sharing, education and training needs, and other technology infrastructure needs. The general workshop structure is described in Section 3, and the workshops are summarized in Section 4.

To ensure Road Map outcomes focused on industrial separations needs as exemplified in Table 1 below, effective collaboration and a multidisciplinary, cross-technology understanding of the problem was maintained. This ensured representative coverage across a range of industrially relevant separation needs (e.g., alkene–alkane) and anticipated potential future chemical processes where water is the solvent. Road Mapping defined critical RD&D projects while identifying opportunities for best practices, tools, and guidance. This information is useful to industrial practitioners who desire to implement Road Map outcomes, and it helps to highlight synergies with emerging separations, such as separations from fermentation broths or similar bio-based and renewable chemical production operations, recovery of valuable dilute components from waste streams, and membrane separations at the natural gas wellhead.

Draft Road Map outcomes from the first three workshops were presented to the separations community at the 2016 AIChE Annual Meeting. The review by this community provided additional information that was used to expand the Road Map direction and helped build the AltSep community of practice. Final Road Map outcomes are provided in this report.

TABLE 1

Priority Distillation Tasks[1,2,3,4]

Olefin/paraffin (e.g., ethylene/ethane) via cryogenic distillation
Crude tall oil fractionation
Azeotrope/water (e.g., IPA/H_2O, Vinyl Acetate/H_2O)
Aromatics (e.g., ethylbenzene/ styrene, ethylbenzene/xylene)
Cumene/phenol
Recovery of dilute organics from water: Current base (e.g., MeOH/H_2O, H_2O/HOAc) New capacity (e.g., carboxylic acids via fermentation/H_2O)
Polyols (e.g., ethylene glycol/propylene glycol)
Natural gas cryogenic distillation (e.g., N_2/NG, C_2/C_3/C_4)
Crude oil and fuel fractionation
Oxygen from air via cryogenic distillation

1. ORNL, 2005. *Materials Research for Separation Technologies.*
2. Humphrey and Keller, 1997. *Separation Process Technology.*
3. DOE ITP, 2005. *Hybrid Separations/Distillation Technology.*
4. AltSep Workshop 1, 2016.

Phase 3— Ensure adequate follow up

This Road Map is intended to provide suggestions to research funding organizations (e.g., NSF, DOE, NSF SBIR) about low-energy separations RD&D funding needs. The ACS GCI Industrial Roundtables are interested in tracking progress of these projects, both to advocate for funding to translate project findings into useful tools and best practices, and to distribute such tools and best practices through the ACS GCI web portal to make them readily available. The Roundtables plan to monitor and recognize developments (e.g., simulation tools) from research projects related to needs identified in the Road Map.

To ensure lasting impact of this Road Mapping project, the AltSep steering team continues to engage the network of AltSep workshop participants; examples of this engagement include AltSep-related programming at the yearly ACS Green Chemistry & Engineering conference and the AIChE Annual Meeting. In doing so, the steering team seeks to identify opportunities to promote Road Map implementation.

3. General Workshop Structure

Each workshop began with general background presentations to seed subsequent discussion and frame the workshop objectives. For Workshops 1–5, outcomes were developed through a series of facilitated discussion sessions among 30 or more participants to identify and prioritize RD&D projects. Participants were asked to brainstorm answers to targeted questions developed by the AltSep team. Notecards were provided to participants, who used them to respond to the targeted questions. After brainstorming was completed, participants were asked to vote on the projects that would have the greatest significance and impact. Those projects garnering six or more votes were considered priority projects and used for subsequent analysis of the workshop results. During Workshops 2–5, a limited number of small groups developed project plan worksheets around the highest-ranked project ideas collected from workshop participants during the facilitated sessions. Workshop 6 convened 8 experts and 3 discussion moderators to outline a path toward molecular properties-based design of polymer membranes. This workshop proceeded through a series of presentations followed by facilitated discussion and brainstorming sessions.

4. The Road Mapping Workshop Process

4.1 WORKSHOP 1: Identifying Key Properties for Separations

FEBRUARY 17–18, 2016

Workshop Participants are listed in Section 6.1

Workshop 1 assembled a diverse group of separations researchers and practitioners. It provided an opportunity for the AltSep steering team to (a) compare different methods for obtaining expert opinions on separations needs and (b) collect valuable input for the Road Map. It was devoted to unearthing molecular-based and other properties that might be utilized to develop novel separations approaches. Part II of the workshop focused on the thought process that might be used for selecting separation alternatives, other than distillation, for industrial-scale separations processes.

- Table 2 on pages 14-15 shows an illustrative list of key properties that workshop participants identified. Novel industrial-scale separations processes may potentially exploit these properties.
- Table 3 on pages 16-17 shows the major steps of the separations system selection process.

4.2 WORKSHOP 2: Intrinsic Molecular Properties and Interactions

JULY 14–15, 2016

Workshop Participants listed in Section 6.2

Workshop 2 built out the AltSep Road Map around the intrinsic molecular properties and interactions of fluid mixtures, solid mass separating agents (MSAs), molecules in fluid mixtures when in contact with or near solid MSAs, and the influence of external stimuli on these properties. It focused on separating molecules with molecular weights of less than 750. Prior to the workshop, a vision for the conceptual design of 21st Century separation processes (*see box on page 18*) was crafted to help participants better understand the overall aims of the AltSep Technology Road Map project. Participants identified requirements for several important areas, such as the increased availability of tools for molecular simulation, data validation, the propagation of trusted molecular property databases, and translating molecular properties to physical properties needed for process simulation and design.

TABLE 2

Properties To Be Potentially Exploited for Separations

INTRINSIC MOLECULAR PROPERTIES	MOLECULAR INTERACTIONS	FLUID PHYSICAL PROPERTIES	BULK PROPERTIES
1 Molecule	**≥2 Molecules**	**Many Molecules**	**Many Molecules**
Molecular weight	Pi-bonding	Heat capacity	Magnetism
Molecular volume	Aromaticity	Heat of fusion	Density
Molecular shape	Dipole interactions including hydrogen bonding	Heat of vaporization	Surface charge-charge density
Molecular size	Inorganic/organic interaction or chelation (e.g., functional groups that can bind to metal) [measured via a binding constant]	Critical properties (T & P)	Crystal structure polymorphism
Molecular charge	Electrostatic interactions	Boiling point	Degree of crystallinity
Quadrupoles and higher poles	Steric interactions	Melting point	Glass transition temperature
Dipole moment	van der Waals interactions	Compressibility	Electrical conductivity
Polarizability			Dielectric constant
Acidity and basicity			Free volume
Moment of inertia			Morphology/surface
Flexibility			Monomer sequence
Degrees of freedom			Viscoelasticity
Chirality			Tacticity
Degree of functionalization			
Electronegativity (including charge delocalization)			

PROPERTIES AT INTERFACES	TRANSPORT PROPERTIES	AQUEOUS SOLUTION PROPERTIES	CHEMICAL REACTIVITY	PHASE EQUILIBRIA
Charge separation	Viscosity	Ionic strength	HOMO/LUMO gap	Octanol/water partition coefficient
Interfacial tension (gas/liquid, gas/solid, liquid/liquid, or solid/liquid)	Thermal conductivity	Critical micelle concentration	Energy-induced reactions (e.g., light, thermal, electrical)	Liquid-liquid equilibria
Self-ordering phenomena (e.g., surfactant interaction or self-assembly)	Diffusivity	Amphotericity	Dynamic properties (change in response to external stimulus — e.g., temperature, pressure, concentration of species, etc.)	Vapor-liquid equilibria
	Membrane-based condensability	Hydrophilicity or hydrophobicity		Solid-liquid equilibria
	Facilitated transportability (membranes)	Salt formation		Synergistic non-idealities (solubility in mixtures — solid/liquid)
	Near-interface transport properties of pure compounds (effect of confinement) on pure species	Solvation structure as a function of composition and concentration		Solubility of solids and liquids in pure and mixed solvents; also as a function of temperature (evaporation, crystallization, liquid-liquid extraction)
	Non-ideal mutual diffusion effects (Maxwell–Stefan phenomena)			Solubility/solubility product/precipitation
				Fugacity coefficients
				Activity coefficients (phase equilibrium estimation)
				Critical activity — solid/liquid and solid/gas
				Solubility parameter (solvent-based separation)
				Solid-vapor equilibria
				Miscibility
				Lyotrophicity

TABLE 3

Separations System Selection

1. Pre-Check of Separation Task	2. Define the SeparationTask	3. Check Feasibility of MSA	4. Find and Catalogue Molecular Property Values	5. Fill in Molecular Data Gaps Through Modeling
• Know your time frame • Know the feed composition boundaries and temperature/ pressure ranges • Review alternative chemical process flow • Is it worth it? Determine cost of doing it • Is there a possibility of retrofitting the existing infrastructure?	• Determine temperature and pressure range the mixture is stable within (or time can be held at temperature/pressure) • Define targets in terms of: ○ Compound(s) ○ Specifications ○ Scale (i.e., throughput) • Process Safety — (T, Z_i) — Can key components be isolated safely in purified form? Consider products and by-products. Evaluate reactive hazards (e.g., DSC) • Determine compatible materials that can contact the feed • Consider the time-sensitive nature of the feedstock	• Supply chain — availability of input materials (MSA) in a sustainable way • Consider thermodynamics of the separation: Determine the $\Delta G_{unmixing}$ for the target from balance of the mixture to help identify least energy consumption for the separation • Feasibility of MSA. R&D needs of manufacture of MSA • Technology, supplier, and input • Identify impact of potential capacity bottlenecks (single train) • Consider development of novel MSA that can work in separating the fluid mixture • Use molecular modeling to help identify parameters for desired new MSA • Integration of required process equipment (e.g., pump, compressor) with proposed unit operations • Confirm membrane module (incl. glues, gaskets) manufacturability	• Search databases for existing data before new measurement or calculation: ○ Chemical properties ○ Physical properties ○ Relevant processes • Find available property data and their reliability, and decide on most important missing data — identify knowledge gaps and whether knowledge needs are critical; need to have reliable properties of mixture and constituents • Collect (literature, experiments, and/or simulation models) molecular properties of key components for separations • Determine properties which define speciation (e.g., concentration, volatility, molecular size, electronic properties) • Rapidly access relevant data on molecular properties (including understanding mixture effects) • Framework to identify which molecular properties are differentiated • Consideration of chemical reactivity of MSA: ○ e.g., reaction/separation ○ e.g., reactive distillation membrane reactors	• If insufficient available information on molecular properties, then conduct molecular modeling. Otherwise skip. • Need thermo-physical data to assess and validate molecular model (might need experiment) • Find suitable predictive modeling techniques • Select molecular model to use • Hierarchy of models to identify molecular properties of each component • Identify basic structural differences of the molecules in the mixture to exploit and capitalize on those differences if possible

System description focused on separation of homogeneous fluid mixtures and did not consider interplay with upstream and downstream operations.

6. Explore Differences in Molecular Properties	7. Identify and Select Unit Separation Operations	8. Scale Up to Process and Screen Initial Unit Process Operations	9. Evaluate Sustainability of Process	10. Complete Design of a Sustainable Separation Process
• Know differences in molecular properties of target vs. non-target components, including intermolecular interaction impacts • Determine/select best physical parameters (molecular) for desired separation (OH ... X-Y bonds, shape/size, $M^{s+}X^{s-}$, complexation/aggregation) • Estimate energy consumption of each alternative previously identified and compare to distillation (ΔGunmixing) • Determine driving force for most efficient separation (akin to VLE for distillation) based on approach in Professor Gani's plenary talk	• Determine feasible separation processes • Decision framework for selection of separation(s) → pick best techniques for separation of components in mixture • Determine anticipated impurities in feed and range of concentrations, including feed pretreatment • Determine pretreatment requirements of associated impurities • Recognize presence of surfactants in mixture—may require completely different approach due to strong interactions not accounted for in molecular property info • Relate property differences to use of MSAs or not • If property difference points to use of MSA, obtain information on molecular interactions between mixture components and MSA	• Separation unit operation fundamental modeling • Understand fundamental transport issues of separation • Framework to "reduce" molecular-level model to higher-level model(s) • Translate into process simulation terms • Screen additional molecular properties, which upon consideration may diminish the apparent attractiveness of the separation unit operation selected in step 7 • Check physical feasibility of effecting separation in the unit operation (including physical properties) • Prepare meaningful process flow sheet using process simulation (e.g., Aspen)	• Determine end-of-life disposal process input into LCA (e.g., ultimate fate of used MSA) • Separations equipment lifetime (replacement frequency); Membranes (fouling), Adsorption Beds, Ion Exchange Columns, etc. • Conduct LCA of process train (with focus on energy and consumables) • Calculate economics—operational and fixed • Understand and reduce risks from contaminants or process upsets • Compare/decide on/revise design (iterative loop)	

A Vision for Conceptual Design of Separation Processes in the 21st Century*

A trained process engineer is assigned to develop an optimal conceptual design for separating a multicomponent fluid mixture. She goes to her computer workstation and answers a series of questions to define the separation task at hand. The engineer specifies the target molecule, the balance of the mixture composition, the operating conditions (T, P) at this point in the overall manufacturing process, the separation criteria (specification for target and other constraints), and the required throughput rate.

The computer system then searches for or simulates (a) pure component intrinsic molecular properties of each component in the mixture at process conditions, and (b) intermolecular interaction parameters for the target with each component in the mixture. Using a collaboratively developed algorithm, the computer provides molecular property information for the mixture in the form of component data and interaction parameters and identifies the top three molecular properties with the greatest difference (between the target and other components) that may be exploited for energy-efficient separation. Where use of a mass separating agent (MSA) is indicated, the computer system provides advice on MSA candidates to be considered based on its evaluation of molecule-MSA interactions. For each output scenario, the computer provides an estimate of the data and simulation accuracy, recommendations on what experiments would most improve data quality (in rank order), and one or more contacts in the AltSep community of practice that can serve as a resource. In cases where multiple separators in sequence are required, the engineer selects the process technology to be used for the first step in the separations sequence and asks the computer system to array the most promising properties for each subsequent separation in turn. She considers potential technological synergies and process constraints when making the selection for those overall separation process sequences to move on to process simulation.

For the candidate separation process sequences, the engineer has the computer translate the molecular property and interaction information into physical property estimations for use in process simulation. Combined with the separation task specifications, these physical property estimations (including corresponding accuracy estimates) are then used by the computer system to simulate each separations flowsheet as the basis for design. Simulation outputs include the separation energy used for the sequence, the calculated $\Delta G_{\text{unmixing}}$ for the separation task, and the corresponding thermodynamic efficiency for the separation process sequence. The output also includes a process sustainability assessment with estimates of capital and operating costs, projections of greenhouse gas and other emissions from the process, and evaluation of imbedded natural resource use and environmental, health, and safety aspects of any MSAs in the process. Where relevant, heat integration is optimized prior to reporting energy use for the process. (In cases when she has information available on the reactor(s) in the process, the engineer has the computer consider heat integration across the reaction and separation units.)

The engineer reviews the process simulation results and schedules a meeting with her computational chemistry and thermodynamics resources to discuss improving the accuracy of influential property estimates. Once the path to resolving those issues is set, she meets with design staff to firm up plans for finalizing engineering design of the optimal process for energy-efficient separation by month end.

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* Prepared by R. J. Giraud (July 12, 2016) with inspiration from "Process Design in the Twenty-First Century", pp. 138−139, *Frontiers in Chemical Engineering: Research Needs and Opportunities* (the Amundson Report), National Research Council, 1988 and based on Giraud, "Toward Sustainable Chemical Separation Processes", presented at 20th Green Chemistry and Engineering Conference, June 15, 2016.

4.3 WORKSHOP 3: Process Simulation, Design, and Scale-up

AUGUST 10–11, 2016

Workshop Participants listed in Section 6.3

Workshop 3 focused on adsorbents and membrane materials for solid MSAs, developing effective process simulation tools, metrics for solid MSA-based processes, further understanding solid MSA-based processes' synthesis and conceptual design, issues with scaling up solid MSA-based separation processes, and identifying other projects and training materials for designing and using solid MSA-based separation processes. Workshop 3 also examined commercializing the technology to ultimately affect industry's approach to separations design. Deep analysis of the highest-priority projects resulted in a project plan to provide more detail about RD&D activities and steps to be taken, potential benefits, project timeline, and more. In a separate session, participants outlined a plan for the conceptual design of an adsorption and/or membrane-based process for an assigned separation task.

4.4 WORKSHOP 4: Applied Fields and Their Effects on Separations

FEBRUARY 2–3, 2017

Workshop Participants listed in Section 6.4

Workshop 4 focused on applied fields' potential for reducing the energy intensity of high-throughput industrial separation processes for small molecules (MW<750). Applied fields hold some promise in two ways. In some cases, the external field (e.g., magnetic, electric, light, acoustic, and flow fields, and their combinations) may act on the molecules in the fluid. In others, the external field may influence the behavior of MSAs such as adsorbents (e.g., colloids, particles, meta-materials, macroscopic sorbents), membranes, and ionic liquids. Applied fields are usually used in analytical-scale separations rather than industrial manufacturing processes, so chromatography was considered for throughputs ranging from lab analysis to large industrial-scale separation processes in order to shed light on possibilities for commercializing applied fields and/or applied field-stimulated materials for industrial separations. Workshop participants considered matrices of analytical scale separations processes (based on molecules' inherent properties, interactions, transport phenomena, aqueous phase, and phase equilibria phenomena) to generate ideas for potential analogous industrial scale separation technologies with the goal of identifying and prioritizing RD&D projects needed to understand and routinely use applied fields in low-energy, high-throughput industrial separations.

4.5 WORKSHOP 5: Small Molecule Recovery from Dilute Aqueous Systems

MAY 24–25, 2017

Workshop Participants listed in Section 6.5

Preceded by an Industry Listening Day sponsored by the Bioprocessing Separations Consortium — a National Labs (BioSepCon) initiative to ensure inter-laboratory collaborations and cooperation in bioseparations research — Workshop 5 focused for 2 days on building out the AltSep Road Map as it relates to recovering small soluble organics from dilute aqueous solution in petrochemical and biochemical manufacturing processes. It identified and prioritized ideas for projects to overcome practical and fundamental barriers to widespread application of sustainable alternatives to distillation when separating organics from dilute solution.

4.6 WORKSHOP 6: Design of Nonporous, Amorphous Polymeric Membranes

OCTOBER 27–28, 2018

Workshop Participants listed in Section 6.6

Workshop 6, the final one, took place prior to the 2018 AIChE Annual Meeting. It convened a select group of leaders from industry and academia to outline a path to in-silico design of nonporous polymer membranes for molecular separations from a given liquid mixture. Each participant made a presentation on personal current molecular separations-related research and contributed to collaborative discussions defining what would be required in order for atomistic simulation to provide both enough insight for rational molecular design of amorphous, nonporous polymers and successful, integrated process design. The workshop had two aims:

- Identify specific experimental data and techniques that would enable effective and efficient simulation across length and time scales.
- Describe advances needed to design at the molecular level novel, efficient, amorphous, nonporous polymers and polymer membranes.

5. Summary of Workshop Results

Table 4 provides a summary of the top-ranked concepts based on the project cards from Workshops 1–5. Clearly, modeling and simulation was a recurring theme that ranked very highly across most of the workshops. In addition to taking this ranking at face value (i.e., that modeling and simulation is extremely important), the high ranking may also be an indication of participant's interests and/or the prominence of modeling and simulation in Chemical Engineering today. Regardless of the reason, the project card ranking suggests that modeling and simulation — along with the computational infrastructure, software, and supporting data — are key elements of the Technology Road Map. It is interesting to note that project cards for experiments and experimental approaches were clearly not as prominent as modeling and simulation. This could once again be an indication of workshop participant preferences, or it could point to a very real gap: i.e., laboratory research to experimentally develop molecular property and interaction data for the systematic design of alternatives to distillation is effectively nonexistent.

A second way to look at the relative importance of the project card rankings is found in Table 5, Part A, where the top 6 concept areas are ordered by the total number of top-ranked cards for each concept area and as a percentage of the total number of project cards. A related ordering is shown in Table 5 Part B, where two

TABLE 5

Top Primary Concept Areas and Groupings

PART A **Top 6 Primary Concept Areas**	**Total Project Cards**	**Percent of Total**
Modeling and simulation	38	19%
Methods and tools	20	10%
Data and databasing	20	10%
Standardization	18	9%
Experiments	17	8%
Experiments and models	16	8%
TOTALS	129	64%

PART B **Primary Concept Area Groupings**	**Total Project Cards**	**Percent of Total**
Novel materials, technology and technology development	19	9%
Theory, theories and experiments, and theories and models	13	6%
TOTALS	32	15%

TABLE 4

Top-Ranked Primary Concepts from Workshop Project Cards

TOP-RANKED PRIMARY CONCEPT	**Workshop 2: Molecular Properties and Interactions**	**Workshop 3: Process Simulation, Design, and Scale-Up**	**Workshop 4: Applied Fields and Their Effects on Separations**	**Workshop 5: Small Molecule Recovery From Dilute Aqueous Systems**
FIRST	Modeling and simulation	Methods and tools	Modeling and simulation	Standardization
SECOND	Experiments and models	Test center	Experiments	Modeling and simulation
THIRD	Data and databasing	Data and databasing	Methods and tools, novel materials, standardization, technology development, theories, and models	Experiments

additional project concept areas are formed from several related concept areas so that they are of equal significance to the top 6 concept areas. Taken together, these 8 concept areas and groupings account for nearly 80% of the project cards.

A final way of viewing the workshop output is in terms of the project planning worksheets developed by small groups of workshop participants. As can be seen in Table 6, the top primary concept areas are contained within 4 headings, the largest of which is for novel technology. In some respects this may seem to be a somewhat surprising outcome, given that novel materials, technology, and technology development only accounted for 9% of the project card total. However, novel technology is an enabler of separations alternatives; without new technologies, alternative separations will not become a reality. In addition, the worksheets represent a bias on the part of the workshop organizers toward development, demonstration, and implementation, all of which are clearly industrial drivers.

On the basis of these groupings and a detailed review of the highest-rated project cards, 9 key areas for research, development and demonstration were identified, as seen in Figure 4.

TABLE 6
Top 4 Primary Concept Areas From Project Worksheets

Top Primary Concept Areas	Total Project Worksheets	Percent of Total
Novel technology	10	25%
Modeling and simulation	5	13%
Experiments and models	3	8%
Characterization	3	8%
TOTALS	21	54%

FIGURE 4
Key Research, Development, and Demonstration Needs

6. Workshop Participants

6.1

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