A RESEARCH AGENDA FOR TRANSFORMING SEPARATION SCIENCE:

A YEAR IN REFLECTION

In June 2019, the National Academies of Sciences, Engineering, and Medicine (the National Academies) released the report *A Research Agenda for Transforming Separation Science*[1] that recommended fundamental research that could increase knowledge of how complex mixtures can be separated in a controlled manner and, therefore, advance separation science. Over the past year, exciting research has been published, and conferences have stimulated important conversations on how to advance the field. Here, a brief overview of the report, some highlights from recent research, and some information on recent and upcoming conferences are provided.

REPORT OVERVIEW

The research agenda described in the report focuses on two major themes: designing separation systems that have high selectivity, capacity, and throughput (Theme 1), and understanding temporal changes that occur in separation systems (Theme 2). The report recommends several research directions for each theme that were motivated by challenges and opportunities recognized by the committee.

For Theme 1, the committee identified the biggest challenge as being able to understand and design separation systems for complex mixtures under realistic conditions and emphasized that addressing this challenge is key to transforming separation science. A second challenge was seen as a need to explore a wide array of multiple forces, entropic strategies, cooperative binding mechanisms, and chemical transformations and to investigate new ways to determine and control differential rates of species transport to facilitate separations. A third challenge arose from the reality that most separations involve an interface or interfacial region. The advent of surface-sensitive spectroscopic tools provides an opportunity to probe the molecular structure and dynamics of all types of interfaces that are present in separation systems. The knowledge gained from those studies would open the possibility of designing and controlling the interface to facilitate separations. A fourth challenge relates to the external forces that can cause physical changes in a separation material, changes that can affect the affinity of species for that material. Understanding those phenomena presents the possibility of controlling the structure of separation materials to allow better control of molecular separations. These challenges led the committee to recommend the research directions for Theme 1 shown in Figure 1.
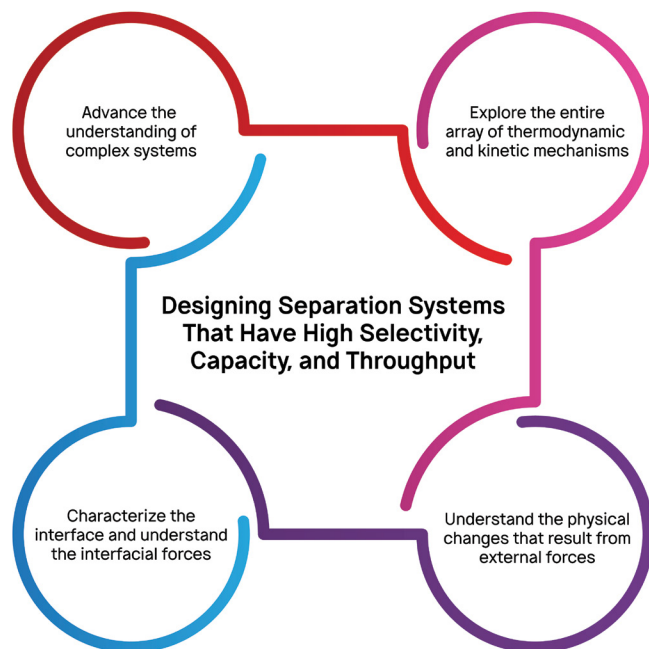

Figure 1
Research directions for Theme 1 of the committee's research agenda.

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For Theme 2, the research directions centered on understanding the factors behind and the origins of chemical, physical, and structural changes to separation materials over time with use. Three common factors that cause separation materials to change are the evolution from a nonequilibrium or metastable state toward an equilibrium state, various chemical reactions that affect the separation system, and interactions of the separation system with unwanted species in the mixture. Understanding those factors would allow separation systems to be designed to be robust in the presence of complex environments and thus formed the basis of three research directions recommended for Theme 2 (see Figure 2). The other research direction for Theme 2 relates to the development of adaptive systems.

The report also identified two cross-cutting concepts—the need for standard systems, samples, and methods and the need to incorporate data science, molecular modeling, and simulation. The committee recommended that the National Institute of Standards and Technology, in cooperation with the research community, identify materials and testing protocols for each type of separation material or system that can be used as reference standards. The committee also recommended that the research community use data science, modeling, and simulation with experimental measurements to develop a fundamental understanding of separation materials in complex environments and at multiple scales.

Implementing the research agenda will require the reinvigoration of a vibrant separation-science and engineering community that can work together to train a new generation of separation scientists and take advantage of advanced experimental and computational tools. Every opportunity to improve interactions between researchers in chemistry and chemical engineering should be pursued,
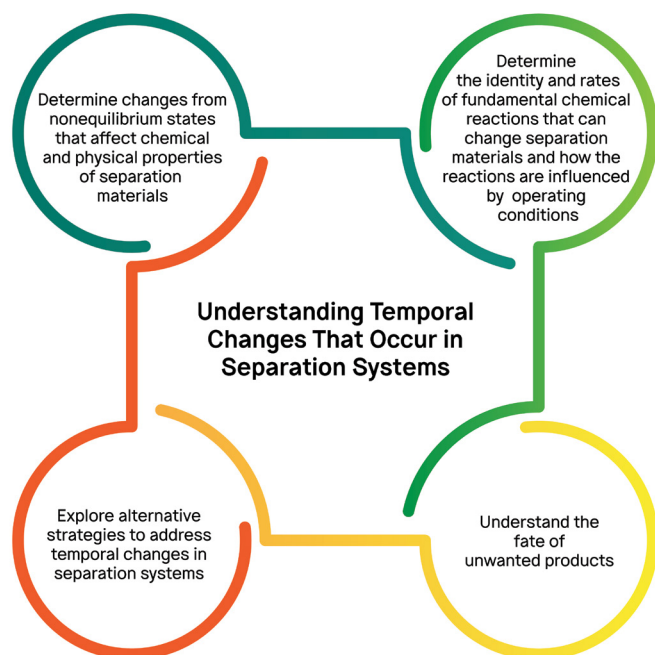
and collaborative projects with a wide variety of disciplines beyond chemistry and chemical engineering will be critical in the new era of separation science. The committee concluded that the research directions identified in this report could transform the way in which separation systems are designed and, if successfully implemented, could ultimately lead to greater U.S. economic competitiveness, a more sustainable chemical-manufacturing ecosystem, and improved human health and the environment.

SEPARATION RESEARCH

Over the past year, many exciting examples of research related to the directions described in the National Academies report have been published. A few illustrative highlights are provided below.

Tracking Particles through Complex Polymer Membranes

Microfiltration (MF) and ultrafiltration (UF) play vital roles in many areas of water purification and biotechnology. A recent review of progress in these separations (Chew et al. 2020) emphasized the empirical nature of approaches that are currently used to assess and reduce fouling in MF and UF membranes and the urgent need to develop fundamental understanding of these phenomena. A fascinating recent example of progress toward this goal comes from coupled experiments and electrohydrodynamic models that track progress of individual solute particles through commercially available polymer membranes. Sorci et al. (2020) showed that simulations could accurately describe the motion of well-characterized silica spheres through porous (poly)ether sulfone membranes and yield quantitative insight into the role of isolated "majority pores" in these complex, disordered materials. The same kinds of simulations were then used to model a hypothetical membrane made with a highly controlled, complex set of interconnected pores. The demonstrated ability to make meaningful predictions about hypothetical pore geometries opens up many possibilities in considering the enormous range of membrane microstructures that are conceivable and driving future synthetic efforts.

Chew, J.W., J. Kilduff, and G. Belfort. 2020. The behavior of suspensions and macromolecular solutions in cross-flow microfiltration: An update. J. Membrane Science 601:117865.

Sorci, M., C.C. Woodcock, D.J. Andersen, A.R. Behzad, S. Nunes, J. Plawsky, and G. Belfort. 2020. Linking microstructure of membranes and performance. J. Membrane Science 594:117419.

Achieving Selectivity through Hierarchically Porous Polymer Nets

Strategies for the design of selective adsorbents tend to focus on development of highly ordered materials, such

Figure 2
Research directions for Theme 2 of the committee's research agenda.

as metal organic frameworks and zeolites, that contain uniformly precise pores and can separate adsorbates on the basis of small differences in size, chemical affinity, and other factors. However, design rules for achieving selectivity in more complex materials that have diverse pore sizes are less well established. Chakraborty et al. (2019) demonstrated a hyper-cross-linked hierarchically porous organic polymer that is highly selective for xenon separation from various gas mixtures, including such similar noble gases as krypton. These porous organic polymers are simple to make, have tunable pore sizes and surface area, and display robust chemical and thermal stability. Although they are much more disordered than traditional adsorbents, these polymer nets have enough functionality within the pores to control the proximity and degree of overlap from multiple polymer atoms to achieve highly favorable host–guest interactions. These versatile materials offer interesting opportunities to combine the advantages of disordered polymers that are widely exploited in membranes that are used in separations based on adsorption.

Chakraborty, D., S. Nandi, M.A. Sinnwell, J. Liu, R. Kushwaha, P.K. Thallapally, and R. Vaidhyanathan. 2019. Hyper-cross-linked porous organic frameworks with ultramicropores for selective xenon capture. ACS Appl. Mater. Interfaces 11(14):13279-13284.

Exploring Protein–Polymer Interactions Using Single–Molecule Spectroscopy

Protein separations are highly influenced by conformational changes and dynamics of proteins at polymer interfaces. An understanding of the microscale packing of polymers and protein dynamics at polymer films provides the opportunity to modify polymer surface chemistries to control protein surface interactions. A recent study reports the use of single-molecule spectroscopy (Moringo et al. 2020) to probe the dynamics of two oppositely charged proteins—α-lactalbumin and lysozyme—on the interface of uncharged polystyrene films of varying free volume. The tracking results revealed that each protein exhibited different adsorption-desorption behavior at the polystyrene surface, with lysozyme exhibiting non-Brownian surface transport that depended on the free volumes among the polystyrene chains in the polymer film. It was shown that the polystyrene film could be doped with a hydrophilic polymer to examine short-range interactions and that ionic conditions could be varied to evaluate the role of electrostatic forces in protein dynamics at polystyrene surfaces. The single-molecule approach provides an insightful means to examine nanoscale protein dynamics at polymer interfaces and characterize important interfacial forces.

Moringo, N.A., H. Shen, L.J. Tauzin, W. Wang, and C.F. Landes. 2020. Polymer free volume effects on protein dynamics in polystyrene revealed by single-molecule spectroscopy. Langmuir 36(9):2330-2338.

Open Sesame: Unraveling the Secrets of Liquid–Liquid Interfaces in Solvent Extraction

Liquid–liquid interfaces are the gate keepers of mass transfer in solvent extraction separation systems. Recently, the research community has begun to embrace a comprehensive approach to characterizing interfaces that are actively undergoing separation events and is beginning to understand solute transport mechanisms and their associated thermodynamic and kinetic features. Research includes multimodal studies that use surface sensitive sum frequency generation spectroscopy with X-ray reflectivity and grazing incidence X-ray diffraction, complemented by molecular dynamics simulation, to study solvent extraction. Liang et al. (2019) has worked to characterize the interfacial structure and species that exist immediately adjacent to a fluctuating and heterogeneous liquid–liquid interface. In their study, a series of metal ions being transported were correlated with different transport mechanisms and a growing understanding of the connection between the observed interfacial structure and the extraction mechanism. Background ions in the aqueous solution are also being demonstrated to have an important effect on mass transport efficacy and solute selectivity in solvent extraction systems, as shown by Lovering et al. (2020). There, comparisons of the adsorption behavior of nitrate and thiocyanate indicated that background ions can influence the water structure at the interface and thus potentially influence extraction mechanisms. Relating those observations to the underlying free-energy landscape of mass transfer is a substantial challenge; simulation methods must use multiple approaches to understand the ensemble of transport processes and how they are related to solvation and interfacial structure as modulated by solution conditions. Recent work in the laboratories of Benjamin, Morita, and others are working to identify the proper reaction coordinates for solute transport—with an emphasis on facilitated ion transport—as a first step toward mapping the underlying energy landscapes (Benjamin 2019; Koizumi et al. 2020). Although it is system-dependent, the ability to map the energy landscape and to understand the barriers and collective rearrangements of the interface during transport is beginning to pave the way toward design principles for solvent extraction that use the interface for advantageous mass-transfer properties.

Benjamin, I. 2019. Hydronium ion at the water/1,2-dichloroethane interface: Structure, thermodynamics, and dynamics of ion transfer. J. Chem. Phys. 151:094701.

Koizumi, A., H. Tahara, T. Hirano, and A. Morita. 2020. Revealing transient shuttling mechanism of catalytic ion transport through liquid–liquid interface. J. Phys. Chem. Lett. 11(4):1584-1588.

Liang, Z., W. Bu, K.J. Schweighofer, D.J. Walwark Jr., J.S. Harvey, G.R. Hanlon, D. Amoanu, C. Erol, I. Benjamin, and M.L. Schlossman. 2019. Nanoscale view of assisted ion transport across the liquid–liquid interface. PNAS 116 (37):18227-18232.

Lovering, K., S. Nayak, W. Bu, and A. Uysalet. 2020. The role of specific ion effects in ion transport: The case of nitrate and thiocyanate. J. Phys. Chem. C 124(1):573-581.

RECENT CONFERENCES

ILSEPT – 4th International Conference on Ionic Liquids in Separation and Purification Technology
September 8–11, 2019, Sitges, Spain

At this meeting, researchers discussed their cutting-edge results on the use of ionic liquids in separation applications. See https://www.elsevier.com/events/conferences/international-conference-on-ionic-liquids-in-separation-and-purification-technology.

2020 Gordon Research Conference on Chemical Separations: Separations Breakthroughs for Commodity and Specialty Chemicals, Environmental Science and Analytical Chemistry
January 26 – 31, 2020, Galveston, TX

This new Gordon Research Conference (GRC) brought together separation scientists from diverse fields to share fundamental advances and was a direct result of the National Academies report, inasmuch as it was proposed and organized by two committee members. Although there were GRCs on separation and purification, which began in 1952, the last in that series occurred in 2000. The next in the new GRC series will focus on fundamental science and take place in Spring 2022. See https://www.grc.org/chemical-separations-conference/2020/.

Pittcon2020
March 1–5, 2020, Chicago, IL

Pittcon brings together experts to discuss the cutting edge of laboratory science. This year's conference featured hundreds of talks on separation science and numerous separation equipment exhibitors. See https://pittcon.org/pittcon-2020/.

UPCOMING CONFERENCES

International Congress on Membranes & Membrane Processes 2020
December 6–11, 2020 | ExCel London, London, UK

This conference will bring together experts in membrane science to exchange new findings and developments in membrane science and will focus specifically on technology, fundamental applications, and emerging trends in how membranes are being used in the field and in industry. See http://www.icom2020.co.uk/.

Actinide Separations Conference
Postponed to May 18–20, 2021

This conference will focus specifically on new and changing forms of actinide and fission product separations, from essential processes to recovery of products and waste management. See https://pnnl.cvent.com/events/actinide-separations-conference/event-summary-a4b9b9b73b0c4fa7a397b-3f132b6dd4f.aspx.

29th Rare Earth Research Conference (RERC29)
Postponed to June 20–24, 2021

RERC29 will bring together a range of experts to discuss a broad array of topics that pertain to rare earth metals, including separations as it relates to such critical materials as actinides, lanthanides, and more. See http://web.sas.upenn.edu/rerc29/.

International Solvent Extraction Conference
Postponed to September 26–October 1, 2021

This conference will explore the scientific and engineering aspects of solvent extraction, with the goal of promoting research, coordination, and new applications of the technology. See https://isec2020.com/.

HPLC2020, San Diego, CA
Postponed to 2022

The International Symposium on High Performance Liquid Phase Separations and Related Techniques invites scientists, industry experts, and policy-makers to discuss the latest in liquid-phase analytical separations. Attendees will exchange ideas, innovations, and best practices on new separation technologies and their applications in medicine, biology, environment, manufacturing, fundamental science, and more. A plenary session will include a presentation of the National Academies report that focuses on unmet needs in separations, funding opportunities, and academic industrial collaborations. See https://www.hplc2020-usa.org/index.html.