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A Research Agenda for Transforming Separation Science

Committee on a Research Agenda for a New Era in Separation Science

Board on Chemical Sciences and Technology

Division on Earth and Life Studies

Motivations for Study

- A vision and strategy for separation science last offered by National Academies in 1987 report, *Separation and Purification: Critical Needs and Opportunities*.

- Some dramatic successes in separation science over the last few decades, but fundamental challenges remain.

Compelling Reasons to Undertake Study

- Develop a sustainable chemical enterprise to drive the economy.
- Reduce adverse effects of industrial activities.
- Improve human health.
- Address new and challenging separations.
- Opportunities for a paradigm shift.

Statement of Task

Develop an agenda for fundamental research in separation science.

- Assess recent research efforts to advance separation science and identify advances in other fields that might be relevant to separation science.

- Identify needs and opportunities for novel instrumentation and educational and human-resource needs.

- Assess potential impacts that fundamental research in separations can have on industrial practices and technology.

Committee

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Committee's Approach to Task

- Focused on chemical, analytical, and biological separations, but excluded separations involving organelles, cells, and viruses.
- Excluded mechanical and physical separations and mature technologies, such as distillation and evaporation.
- *Focused on a fundamental research agenda, not an empirical investigation of particular processes.*

Research Agenda

- Committee identified two research themes and eight research directions.
- Committee views each research direction as a recommendation for study and exploration.
- *Committee did not set priorities for research directions because advances in no single research direction will be sufficient to transform the field as a whole.*

Research Themes

- Theme 1: Designing separation systems that have high selectivity, capacity, and throughput.
- Theme 2: Understanding temporal changes that occur in separation systems.

Theme 1: Research Directions

Advance the understanding of complex systems.

- Develop measurement and simulation techniques for multicomponent mixtures.
- Design separation systems that can handle a large dynamic range.
- Advance trace analysis and multistep processes.

Theme 1: Research Directions

Explore the entire array of thermodynamic and kinetic mechanisms.

- Explore a broader variety of multiple forces, entropic strategies, and cooperative binding.
- Design for recycle and reuse.
- Explore a wide array of chemical transformations to facilitate separations.

Theme 1: Research Directions

Characterize the interface and understand interfacial forces.

- Surface-sensitive experimental spectroscopic tools can now probe the structure and dynamics of all types of interfaces at the molecular level.

- *That ability opens the possibility of designing and controlling the interface and interfacial region to facilitate separations.*

Theme 1: Research Directions

Understand the physical changes that result from external forces.

- External forces can cause physical changes in separation materials, which can affect the affinity of species for those materials.
- *Those phenomena, if understood, present the possibility of controlling the structure of separation materials on length scales that allow better control of molecular separations.*

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Theme 2: Research Directions

Determine changes from nonequilibrium states that affect the chemical and physical properties of separation materials.

- Understanding aging mechanisms and what controls the rate of change toward lower-energy confirmations allows the possibility of purposefully synthesizing nonequilibrium phases and controlling their evolution.

Theme 2: Research Directions

Determine the identify and rates of fundamental chemical reactions that can change separation materials and how the reactions are influenced by operating conditions.

- That information can be used to identify strategies to prevent degradation from unwanted chemical reactions.

Theme 2: Research Directions

Understand the fate of unwanted products.

- Understanding the interactions of degradation products, the relevant phase equilibria, and the fundamentals of nucleation and growth will allow better design of separation materials at an early stage of discovery and testing.

Theme 2: Research Directions

Explore alternative strategies to address the temporal changes in separation systems.

- ➢ Adjust operating conditions or use additives.
- ➢ Explore planned degradation.
- ➢ Design materials to be self-healing.

Cross-Cutting Issues

Standard Systems, Samples, and Methods

Recommendation: The National Institute of Standards and Technology, in cooperation with the research community, should identify materials and testing protocols for each type of separation material or system that can be used as reference standards.

Cross-Cutting Issues

Adapting Theory and Data Science for Separations

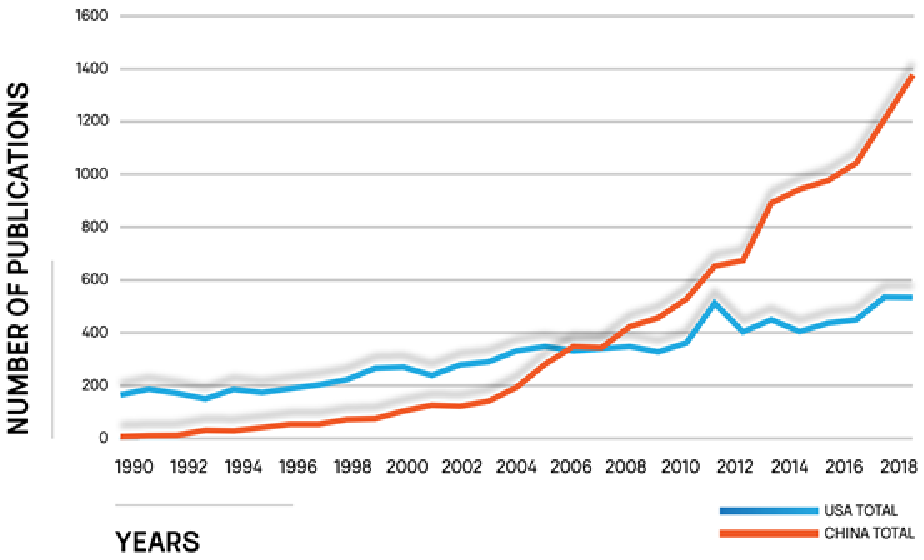
Recommendation: The research community should use data science, modeling, and simulation with experimental measurements to develop a fundamental understanding of separation materials in complex environments and at multiple scales.

Implementing the Research Agenda

Implementing the research agenda will require a reinvigoration of a vibrant separation-science and engineering community who will work together to train a new generation of separation scientists.

Challenges to Implementation

Is the United States losing its competitive edge in separation science?



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Challenges to Implementation

- Decreasing trend in the number of separation-science faculty in the United States – 40% decrease in top analytical chemistry programs and 30% decrease in top chemical-engineering departments since 1987.

- Undergraduate courses are not conveying the excitement of new advances in separation technology.

Overcoming Challenges

Recommendation: Because separation science is integral to chemistry and chemical engineering, these academic departments should provide high-quality training in separations.

Recommendation: The chemistry and chemical engineering separation communities should seek opportunities for substantive interactions that will inspire creativity and the integration of concepts in research and education.

Leveraging Discoveries and Tools from Various Disciplines

Multidisciplinary, multi-investigator collaborations will be needed to perform all the theoretical, computational, and experimental research needed to advance the frontiers.

***Recommendation**: Federal agencies should promote cross-fertilization of separation researchers from intersecting disciplines and encourage collaborative projects as a key priority.*

Impact on Industrial Practice

Replacing familiar, established separation systems with new technology requires a high level of confidence and reliability, and implementation of the research agenda will be critical for reducing risks associated with the adoption of next-generation separation technologies by industry.

Concluding Remarks

- The key research directions identified in this report will transform the way in which separation systems are designed.

- If successfully implemented, the transformation of separation science could affect analytical-scale and process-scale industries and lead to greater U.S. economic competitiveness, a more sustainable chemical-manufacturing ecosystem, and improved human health and environment.