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Editorial

Transforming Separation Science for Improved Human and Environmental Health and Addressing the Fundamental Challenges in Separation Science

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EDITORIAL

Separation science plays a vital role in maintaining our standard of living and quality of life. Most of the industrial processes and general necessities such as chemicals, medicines, clean water, safe food, and energy sources rely on chemical separations. However, the process of chemical separation is often overlooked during product development and this has led to inefficiency, unnecessary waste, and lack of consensus among chemists and engineers. A reevaluation of system design, establishment of standards, and an increased focus on the advancement of separation science are imperative in supporting increased efficiency, continued manufacturing competitiveness, and public welfare.

In recent decades, the technology and chemistry communities have made rapid advances in separation science and technology. To take advantage of these advances in experimental techniques, data science, and computation and simulation, key fundamental challenges in separation science must be addressed. Chemical separations are invaluable processes that underpin diverse chemical transformations. Virtually every product that people use depends on efficient chemical separations. Designing separations that have high capacity, selectivity, throughput and understanding temporal changes that occur in separation systems are the two major challenges. The ability to make molecules and assemblies of molecules that have the desired functional properties is necessary to advance separation science and there are synthesis challenges with making new materials in a form that can be used in a separation system. The importance of synthesis for many disciplines is clearly recognized, as seen in the exploration of the topic by funding and research communities. Additive manufacturing might offer new opportunities to produce structured adsorbents, especially membranes that have improved performance. Standardized systems of materials and testing protocols for separation science and the exploitation of data science to extract new knowledge and insights from large complex datasets are the cross-cutting topics.

Selectivity, capacity, and throughput are arguably the key defining features of separation processes, so developing fundamental approaches that improve performance in these factors lies at the heart of separation science. Many pressing fundamental research issues are associated with the robustness of separation systems. The diversity and complexity of materials and processes that can be used in chemical separations are both signs of the opportunities and a challenge to the research community. The importance of data reproducibility is relevant in all fields of scientific research; separation science is no exception. In principle, data science has the potential to accelerate progress in all aspects of chemical separations. Initial efforts have been made, but the use of data-science methods in chemical separations is nascent at best.

Chemical separations are entering an era in which fundamental advances will be possible. In broad terms, this fertile intellectual landscape will include challenges associated with the intrinsic characteristics of separations and challenges associated with the evolution of separation systems during use. There are large gaps in both areas, and progress in both will be critical for major advances in the field. The difficulties of understanding and controlling the phenomena that appear in complex chemical environments and in situations that span large dynamic ranges should become defining features of fundamental work in chemical separations.

The constant development of MS analytical science has pushed boundaries in the past 20 years. The high throughput required by the bio/pharma industries means that we need not only ever increasingly precise and sensitive systems for quantitative and qualitative analyses, but also speed in acquiring the data. The data also needs to be as comprehensive as possible, providing meaningful information that can be linked with physiology and disease mechanisms. This is imperative, not only for drug discovery in bio/pharma, but also in basic life sciences research, where investigating disease biomarkers and treatment targets is fundamental. It is these novel discoveries and ongoing research and development that are facilitating the realization of precision and personalized medicine today and in the near future.

Much of discovery research now employs a multi-omics approach, looking at the genomics, transcriptomics, proteomics, metabolomics, and other -omics of human health and disease,

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using complex biological samples from humans as well as model systems, available in varying amounts. This means that mass spectrometry using electrospray ionization needs to be performed at different liquid chromatographic (LC) flow rates, such as nanoflow for proteomics, where sample amounts tend to be especially limited, and microflow for metabolomics, where sample amounts are frequently more abundant.

Analytical chemists continue to develop methods for ultratrace-level analyses that are used by practitioners in areas such as environmental, human health studies, and process technology. However, questions continue to arise about whether the current methods are adequate. Global challenges that point to the need for significant disruptive technology in analytical chemistry should be addressed. For example, Endocrine disruptors either mimic or block the production of naturally occurring hormones. Compounds known to be endocrine disruptors include parabens, triclosan, polychlorinated biphenyls, bisphenol A, dioxin, flame retardants, plasticizers, and some pharmaceuticals. For many of these compounds, the minimum concentration level that will not affect the endocrine systems is not yet known. Similarly, oxidative stress on humans and wildlife because of exposure to ultratrace levels of pollutants is also of significant concern. Oxidative stress is suspected in neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, and multiple sclerosis.

Current analytical devices are not meeting all the needs for ultratrace-level detection as described above. We must develop new means to lower the detection limits of organic and biological compounds. Clearly, further improvements in preconcentration capabilities with solid-phase extraction (SPE) and in chromatographic efficiency must occur. These improvements will facilitate improved detection limits for the analysis of small to medium organic compounds. In addition, MS detection limit improvements are needed. Analytical chemists must push forward to move detection limits lower and continue to improve the selectivity of analyses.

It is estimated that poor air quality contributes to almost 500.000 premature deaths across Europe each year. It is important that we identify the compounds in a Particulate Matter to understand its source and possible hazards associated with it which would allow regulators to target the source of the particles and to know specific hazards associated with the particles. Compounds like PAHs occur at incredibly low levels in PM making their determination difficult. Recent advances in Gas Chromatography – Mass Spectrometry are allowing researchers to develop novel, accurate and precise methods in the determination of such compounds.

More predictive, biologically relevant high throughput screening techniques are necessary to improve early stage compound screening. Rejecting compounds early in development based on actionable, high quality safety and efficacy data from assays relevant to the target disease and human physiology will bring substantial benefits by avoiding the much higher expense of failure down the line in human clinical trials.