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COMMENTARY

Six Degrees of Separation: Connecting Research with Users and Cost Analysis

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New scientific developments can benefit society in incredible ways. Tremendous research efforts strive to develop new materials, processes, and techniques to meet challenges of direct relevance to societal and environmental problems. Yet despite best intentions, many technologies developed in research labs either begin or become poorly aligned with the needs of the industry in which they would operate. Of course, the role of academic research is not only to create and commercialize new products. Scientific inquiry aimed at deepening understanding or "blue sky" research without a specific application focus is of paramount importance, as such work benefits and stimulates intellectual curiosity and can also lead to technological breakthroughs. However, for the case of applied academic research, where there is strong motivation to directly impact technology challenges, there is a need for greater interaction with potential users of the technology as well as quantitative assessment and cost modeling. Exploration of customer needs and cost modeling is often disconnected from the research team itself or only initiated after much investment has already been made.

This gap between academic research and commercial viability can be seen particularly clearly through a case study in membrane technologies. Despite hundreds of new proposals for materials, configurations, and methods against fouling, commercially available membranes for water filtration and other applications have largely remained unchanged, with only minor tweaks for nearly three decades.[1] Yet the potential benefits of new membrane materials are enormous. Consider energy utilization: 12% of the annual energy consumption in the United States is due to thermal separation processes, used almost entirely by chemical and petrochemical processing. Ninety percent of this energy would be saved by transitioning to membrane-based separation: 11 quadrillion BTU or $200 billion annually.[2]

Outstanding research on membrane materials continues, and there are excellent recent discussions regarding specific challenges and opportunities.[3] This is an exciting time in membrane materials design, one in which we are witnessing a convergence of atomic-scale control in the synthesis, unprecedented ability to simulate membrane properties, and – crucially – the tremendous intellectual interest in contributing to membrane materials design that now extends far beyond the traditional chemical and mechanical engineering disciplines. For these reasons, we believe it is critical to emphasize the need for tighter integration between research goals, customer discovery, and quantitative metrics for scalability. Here, we share our recent experience in this regard, related to our work on graphene-based membranes that started with idealized simulations[4] and has led recently to a new commercial venture.

This article describes two toolkits that led us to this transition and focused development. When academic research operates in near isolation from these tools, extensive effort may be expended on technology that is not critically needed or cost effective.Combining scalability analysis with over 200 customer interviews not only helps accelerate the transition from academic concept to commercial potential, but also provides an important feedback loop to the research itself.

Tool 1: Cost and Manufacturing Analysis

When our group first published the molecular simulation of graphene as a desalination membrane,[4] industry's assumption was that costs of new material development were prohibitive and that researchers were largely unaware of the true challenges the industry faced. Despite excitement about the 100× increase in permeability afforded by graphene, the true impact of this lever was not well understood. We modeled and quantified the role of permeability in the plant setting and calculated that the energy savings are marginal at best (up to 15% for seawater) due to the economic dynamics of a large plant, a critical need to avoid salt concentration at the membrane's surface, and the second law of thermodynamics.[5]

This analysis suggests that graphene is an impractical feedstock for reverse osmosis membrane manufacture. Synthesis of chemical vapor deposition (CVD) graphene requires extremely high temperatures (900–1100°C typical) and sacrificial high-quality metal substrates. Current retail CVD graphene films on copper substrates sell for thousands of dollars a square foot. While retail prices may not reflect actual production costs and will likely decline in the future, to what extent and on what timescale such reduction will occur remain open questions and requires that initial applications be able to support development costs. With only a 15% energy saving, the market cannot justify a membrane feedstock that could cost orders of magnitude more than the incumbent technology.

And yet, graphene-based desalination literature keeps growing. Figure 1 (top) shows the number of publications, including both journal articles and patents, that contain certain sets of keywords over the period 2010–2016. The data have been normalized in each case to be a percentage of the total publications as indicated. The number of articles with the words "graphene" (G, to refer to CVD graphene) or "graphene oxide" (GO, to refer to chemical exfoliated graphene oxide) + "nanofiltration" (NF) has witnessed a rapid increase by a factor of 2,500% over this 7-year period (from a total of 54 in 2010 to 1390 in 2016 for G and GO combined). In a remarkably short period of time, a completely new material has become a major component of nanofiltration membrane research.

In parallel, the term "scalable" is littered in the scientific literature with no quantitative analysis. While the term scalable can be used to describe a method for which larger sizes can be achieved, it often reflects cost as well. Moreover, the requirements of "scale" are different for different applications. Because any method can ultimately be repeated for larger areas or higher volume production, the critical question is whether it is economical to do so for a given application. The role of manufacturing is divorced from the early assessment of a process or material, but is presented in a way that is potentially damaging to its viability. In the case of graphene membranes, a simple back-of-the-envelope calculation would challenge many of the claims of some hundreds of academic publications. Because the methods to produce G and GO are very different, and create a very different product, the context is important.

As a feedstock for large-area membranes, two metrics apply for G and GO manufacturing: rate and cost. At the lab scale, 1×10^{-6} g of CVD graphene can be produced in about 2 hr (batch production). For the same period of time, 200 g of graphene oxide can be made. Meanwhile, current retail costs for CVD graphene are roughly $80,000/m^2 compared with $15/m^2 for GO (http://www.graphenea.com/). Although the "real" cost of production of each may be lower, using retail prices for comparison captures the economics of supply and demand, which are relevant to commercialization. Meanwhile, considerable efforts to increase the area while decreasing the costs of CVD graphene have enabled its applicability in electronic and optoelectronic applications. Still, roll-to-roll size areas reported are insufficient to provide 40 m^2 per membrane module with volume sales.[6]

When compared with the $10/m^2 production cost for rolled polymer membranes, only graphene oxide can begin to compete for membrane applications, even when assuming some learning and scaling factors. Yet, as seen in Figure 1 (bottom), regardless of whether G + NF or GO + NF, we observe that roughly ~20% of the articles also contain the word "scalable." The fact that G (note: G implies that GO was excluded) and GO nanofiltration publications refer to "scalable" with similar relative frequency is of concern, since graphene oxide to the first order is a much more scalable feedstock (i.e., its production costs benefit from scaling factors such that higher volumes are more economical to produce).

The frameworks that do exist to evaluate scalability or manufacturing are

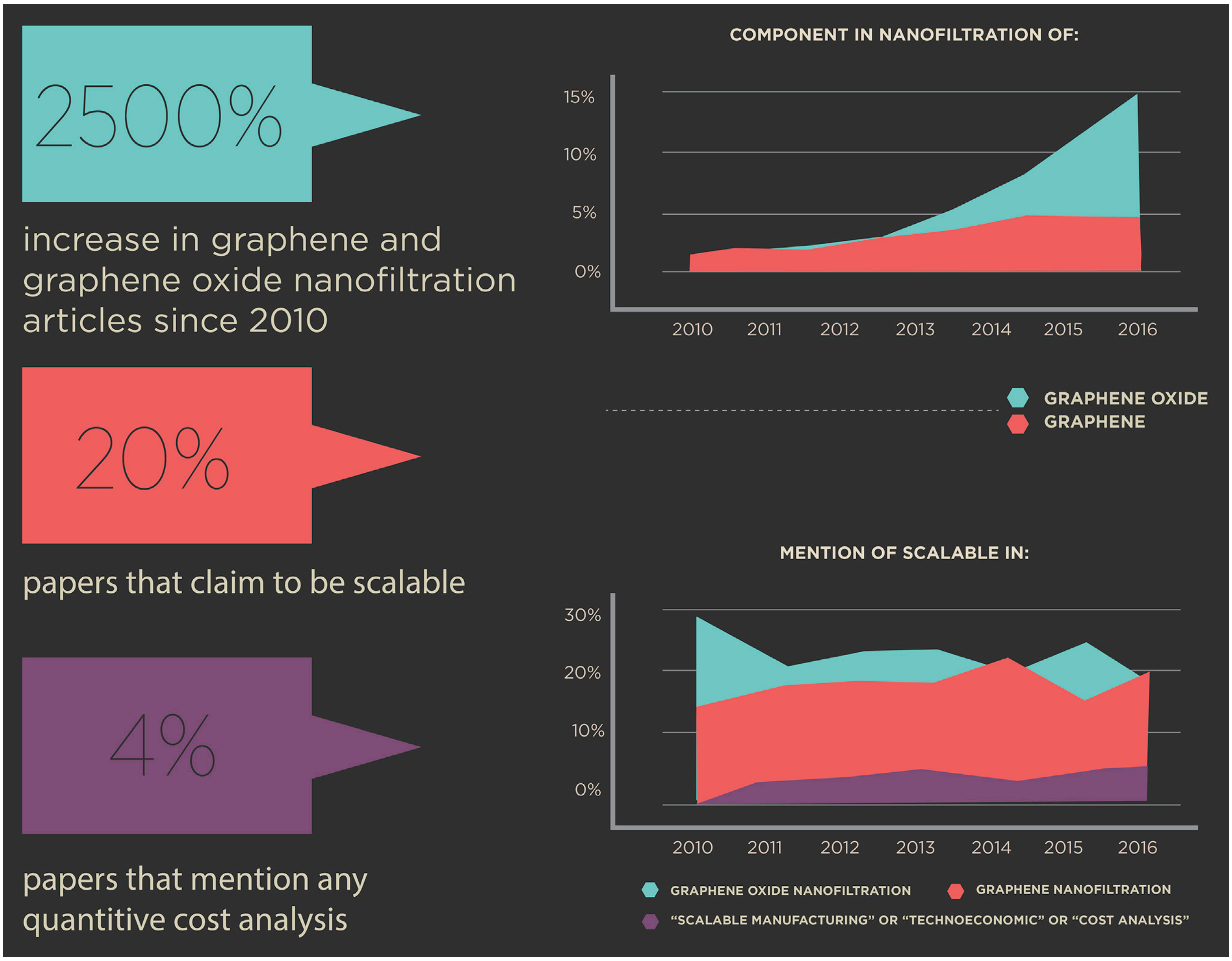

Figure 1. Graphene and Graphene Oxide Membranes in the Literature

(Top) Percentage of occurrences of graphene (G) or graphene oxide (GO) in nanofiltration (NF) research from 2010 to 2016; (bottom) percentage of occurrences of G or GO + NF with and without including the word ''scalable''; and percentage of G or GO with NF and any of the following: ''technoeconomic,'' ''cost analysis,'' or ''scalable manufacturing,'' relative to all NF. All data collected from Google Scholar.

not used frequently enough. In particular, technoeconomic analyses, process-based cost models, and parameter control windows are all relevant at a research stage. If we now seek more specific terms to refer to scalable, including ''technoeconomic,'' ''cost analysis,'' or ''scalable manufacturing,'' we arrive at a much lower percentage of papers, as shown in Figure 1 (bottom). It is interesting to note that the introduction of a small but increasing number of more rigorous cost analyses, which starts at 0 papers in 2010 and rises to 4% by 2016, has no clear effect on the occurrence of the broader ''scalable'' in either the graphene or graphene oxide literature.

It is clear from Figure 1 that while graphene and graphene oxide are extremely ''hot'' areas of research, publishing detailed cost analysis has not been popular, in part because it is historically not a feature of scientific literature. However, the absence of such work has not prevented authors from claiming it as an obvious trait. It is likely that if authors, reviewers, and editors, refused to grant this claim by fiat, that detailed analyses would be more heavily cited, more popular to publish, and the entire community would benefit from better understanding the potential of a technology.

Technoeconomic Analysis

An example of one such technoeconomic analysis follows: reverse osmosis membranes lose their selectivity when exposed to even drinking water levels of chlorine (<4 ppm), and as a result additional steps are required to protect the membrane in a desalination plant, yet membrane fouling remains an issue. By area, a significant fraction of the plant is dedicated to pre- and post-treatments: removing everything else from the water first so as not to foul the delicate membranes and then re-treating the water after it passes through the membrane so it can be sent to a municipal water supply. Even though there are large research programs on the development of chlorine-tolerant polymers for reverse osmosis, understanding of the economic impacts of a chlorine-tolerant membrane remains poorly integrated with the research itself. In fact, we could not find any data to guide how expensive a membrane could be if it exhibited a particular specification. Would it save a plant money if it employed chlorine-tolerant membranes that cost 2 or 10 times the incumbent technology?

To answer such questions, we used the existing Water Treatment Cost Model (WaTER) and updated it for 2016 chemical spot prices, construction indexes, and validated it with the Global Water Intelligence Database. We then calculated the cost of fragile reverse osmosis membranes based on additions to the model for overpressure due to fouling buildup, chemical cleanings including downtime, and de-chlorination and re-chlorination steps. We found that chemical robustness supports about a 2× increase in the price of the membranes. And, in the case of permeability and chlorine tolerance tradeoffs, particularly of interest for a polymer solution, chlorine tolerance supports a 46% reduction in permeability (if cost remains constant). This bounds, but does not preclude, research focused on reverse osmosis membranes, but lends a new perspective to the work. If these industry-facing research programs exist, it is important to consider the technoeconomic facets of the problem.

Process-Based Cost Modeling

Another technoeconomic approach is Process-Based Cost Modeling (PBCM), which converts technical specifications about a product's production process into cost in order to inform technical decisions before investments are made.[7] PBCMs are used at many levels of product development in order to estimate the production cost. The production cost typically has no relation to the prototype cost, and must be calculated with production scale components. For well-established manufacturing methods, a first-order calculation can be conducted using a bill of materials and estimated markup for labor and assembly. For more novel processes, the costs are less certain. The purpose of our quantitative PBCM is 2-fold: first, to determine the potential for commercial application of graphene oxide, and second, to provide early understanding of the cost drivers in order to illuminate the next set of research or development endeavors.

PBCMs from our work and others predict a lower future cost of production for G and GO when compared with the retail costs reported. Our PBCM models eight steps of the production of graphene oxide membranes, including the production of GO, drawing data from unit operations such as agitation and cooling that exist today at scale. Equipment costs are modeled from direct quotes from suppliers, and the feedstock price of chemicals and graphene oxide are marked down from laboratory scale prices to represent bulk purchases. This model suggests that costs will scale with volume with an exponent of 0.6, that the graphene oxide feedstock is not a significant cost driver in the production, and that key process parameters are related to controlling the relative kinetics of film formation and assembly chemistry. This is indicative of scalability in agreement with the empirically derived Viola Method, a well-established scaling factor for chemical engineering processes used to estimate costs at higher volumes based on existing costs.[8]

Process Control Windows

Finally, process control windows, common in process engineering, can also be identified at the earlier stages of research. Even at the bench scale, understanding not only the recipe that creates the optimal results but also the impact of variability in the process creates opportunities for innovation. The greater the variability that the process is able to sustain, the more leverage it has in scale-up economics. Moreover, this enables the researcher to identify process conditions that are most critical and predicts potential failure modes. Together, these analysis methods also allow for assessment of impact, input factors, cost drivers, and equipment specialization.

Tool 2: Interactions with Actual Customers/Users

Given a technoeconomic perspective, what, if anything, then is required of a membrane? We were fortunate enough to participate in the National Science Foundation's I-Corps program in which our mandate was to conduct 100 customer interviews to determine the market viability of the product we had created in the lab. These were highly technical conversations and absolutely relevant to motivating our research. We learned to engage with plant managers and operators, and how to skip past the high-level experts in order to fill out the ecosystem in detail. We spoke to R&D about their research programs, to business developers about their cost requirements, and to customers about their separations needs. We discovered that resilience mattered, just not where we thought it did. We learned that some attributes, like the brittleness of a membrane, may require one threshold for the separation process but a completely different one for the people installing the membrane.

Figure 2 illustrates the landscape of nanofiltration membranes derived from these customer interviews. For these purposes, NF represents the pore diameter regime of 0.001–0.01 μm, or a molecular weight of about 250–1,000 Da. The operating conditions of

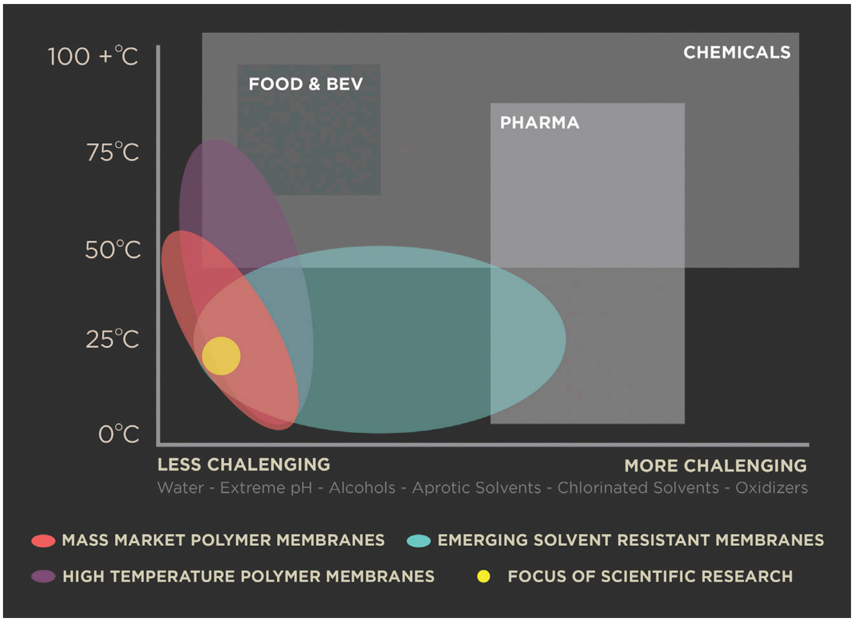

Figure 2. Landscape of Membrane Operating Conditions
The ovals represent the specified operating conditions of commercial nanofiltration membranes today. The boxes illustrate the desires of industrial process separations, based on nearly 200 customer interviews. There is a mismatch between what is available and what is desired, and yet the bulk of academic research is focused on the yellow dot.

commercially available NF membranes is juxtaposed against needs of these industries in Figure 2, showing temperature on the y axis and degree of challenge in chemical environment for traditional membranes. Our now 200 customer interviews reveal that robust membranes could deliver on a massive mismatch between the needs of industrial process separations and the properties of mass-market membranes.

Food and Beverage

Specifically, food and beverage applications suffer from unrelenting fouling challenges. The proteins and sugars that are being fractionated continuously stick on the membrane surface, impeding flow, and requiring increasing amounts of pressure. However, because the membranes are fragile, only gentle cleaning conditions can be used to remove this buildup. In some cases, slow and expensive enzymatic cleans are the only viable method. The labeled box in Figure 2 represents ideal cleaning conditions for food and beverage applications: elevated temperature and pH. Food and beverage presents a unique opportunity for membranes because of inherently fragile product streams for which distillation does not apply; they are high-fouling processes that require resilient membranes.

Pharmaceuticals

Meanwhile, separation needs in pharmaceutical manufacturing include recovering catalysts, active pharmaceutical ingredients, and solvents. For room-temperature applications, solvent-stable polymer technologies have been developed and meet many of the needs in this industry well.[9] Today, these processes are largely batch precipitation, chromatography, and evaporation, and although manufacturing represents a small fraction of the total cost of a drug, throughput-constrained facilities would benefit from solvent-stable membranes that can be sterilized. Efforts toward continuous manufacturing of pharmaceuticals require qualified membranes, and new drug development could be enabled with improved separation capacity.

Chemicals and Petrochemicals

Finally, processes for the chemicals and petrochemicals industries represent nearly all of the energy dedicated to separations and are most reliant on thermal-based processes. The transition to membranes will represent a paradigm shift in the industry and requires significant technological demonstration. Resilience challenges for chemicals and petrochemicals are broad, but these processes are inaccessible to traditional polymer membranes because they almost universally occur at elevated temperature; cooling a stream to pass it through a membrane is almost never capital or energy efficient. Many of these processes are also inappropriate for ceramic membranes because they require separation at the nanoscale. The diversity in application and separation stream is large (see, e.g., Sholl and Lively[2]) and chemical and petrochemical processers will play a significant role in enabling a transition to membranes.

Despite the huge mismatch between the broader conditions at which separations could be performed and the conditions current membrane materials can serve, academic attention is focused heavily on desalination. The looming water shortage is of course a massive global challenge worthy of investment in cutting-edge research, and important science can be motivated from such applications[10]. However, because dialog between industrial users and academic researchers is limited, and because technoeconomic analysis and process modeling is not attractive in proof-of-concept or early work, academic research is investing significant effort in good science that is unlikely to solve the intended problems.

The role of research is multifaceted; research need not be motivated by anything beyond the pursuit of knowledge. But in areas of research focused on direct applications, these two elements are critical. Without more emphasis on customer discovery and technoeconomic analysis, the result is often a bad solution to the wrong problem. Although we are still at the early stages of commercialization in our own work, we would certainly have benefited from using these tools earlier and, based on our lessons learned, genuinely hope that others do too.

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