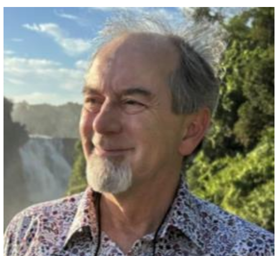
MIT Climate & Sustainability Consortium

Sustainable Separation and Purification of Biochemicals and Biofuels Using Membranes

Project Overview

Building computational tools to accelerate the development of reverse osmosis, an energy-efficient membrane-based process, for the separation and purification of biochemicals and biofuels.


John Lienhard


Nicolas Hadjiconstantinou

Thermal separations processes such as distillation account for over 10% of global energy consumption, typically relying on fossil fuel derived heat. Separation and purification represent 40% of the energy used in producing biomass-derived feedstocks, much of which again depends on energy-intensive thermal distillation. In this project, the team worked to develop new computational tools to determine whether membranes could separate complex mixtures and reduce both the energy and carbon footprint of separations.

The team, led by John Lienhard (Mechanical Engineering), Nicolas Hadjiconstantinou (Mechanical Engineering), and their research groups, including Akshay Deshmukh (Research Scientist) and Runfeng Zhou (Graduate Student), combined thermodynamic models for osmotic pressure in multicomponent mixtures and atomistic simulations of transport across membranes. Their goal was to develop a module-scale computational framework to examine transport across membranes from the pore to system scales. The primary challenge was to extend membrane systems widely used for desalination (water and salt separation) and gas separation (oxygen and nitrogen separation, for example) to multicomponent (more than three distinct chemical species) liquid-phase mixtures.

The project aligns closely with the MCSC's Circularity pathway.

Findings & Outcomes

Highly selective membranes for separating complex liquid mixtures of chemically similar components, common in biofuel and biochemical separations, present one promising path.

One of the key challenges the team identified was that new highly selective membranes must be developed for separating complex liquid mixtures of chemically similar components, which are common in biofuel and biochemical separations. These mixtures require membranes that can exploit small geometric differences between molecules rather than relying on other factors such as charge, which is the dominant mechanism used in water and salt separation for desalination, or solubility, which is widely used in gas separation membranes. The team developed atomistic computational models to conduct the analyses.

Understanding what membrane selectivities (the ratio of rates at which different molecules permeate through the membrane) are achievable and required for industrially relevant mixtures, across a wide range of components, is essential to design new energy-efficient separations. As an example, the project team focused on the highly energy intensive separation of mixed xylenes. Mixed xylenes consist of four structural isomers: ortho-xylene, meta-xylene, para-xylene, and ethylbenzene. Among these, ethylbenzene and para-xylene are critical feedstocks for the production of polystyrene (PS) and polyethylene terephthalate (PET). Each of the mixed xylenes has the same chemical functionality and molar mass, making their separation extremely challenging.

The team demonstrated that achieving sufficient selectivities in this case, for example between ortho- and para-xylene, the latter is a key precursor for PET production requires very fine control over pore geometry. By building system-scale models, the team demonstrated that without sufficient selectivity the number of stages required to achieve effective separation would become large, resulting in increased energy consumption. The new framework the team developed was published and presented at conferences:

- Zhou, Swisher, Deshmukh, Sun, Lienhard & Hadjiconstantinou. "Dense fluid transport through nanoporous graphene membranes in the limit of steric exclusion". *Physical Review Fluids* (2024). (10.1103/PhysRevFluids.9.044202)
- Deshmukh, Zhou, Swisher, Hadjiconstantinou & Lienhard, "Multiscale Modeling of Chemical Fractionation Using Reverse Osmosis". American Institute of Chemical Engineers Annual Meeting (2023)
- Deshmukh, Zhou, Swisher, Hadjiconstantinou & Lienhard, "Multiscale modeling to guide energy-efficient multicomponent separations using membranes," International Congress on Membranes & Membrane Processes (2023)

Opportunities for Implementation

Companies will be able to pilot and implement this research in three ways. First, by identifying which currently energy-intensive separations are best suited for membranes; second, by quantifying the potential energy and carbon savings; and third, by defining the membrane properties required to achieve those separations.

Through in-depth discussions with MCSC members and Impact Fellows, the team was able to analyze key separation bottlenecks in the recycling of ethylene glycol during the production of polyethylene terephthalate (PET). These discussions highlighted opportunities to decarbonize the separation of water and ethylene glycol for PET recycling.

Currently, this separation requires large amounts of heat, typically supplied by process steam generated by natural gas boilers, in distillation columns (see Figure 1). The team's analysis showed that achieving greater than 99.5% ethylene glycol purity, the level required for PET recycling, cannot be accomplished using membranes alone, but membranes can be integrated into an efficiently designed hybrid process that is still electrically powered. This enabled the identification of alternative approaches that are easier to implement, such as coupling membranes with mechanical vapor compression or using heat-pump-integrated distillation in combination with membrane-based processes to achieve a fully electrically powered and energy-efficient separations system.

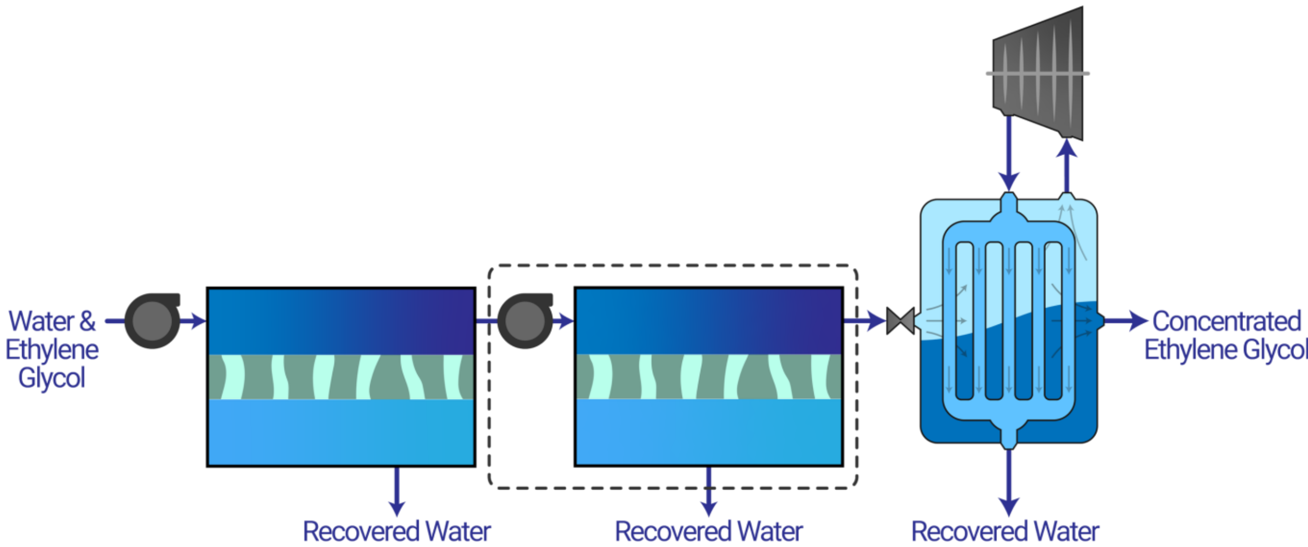


Figure 1: Water and ethylene glycol (EG) separations must reach greater than 99% EG purity for effective polyethylene terephthalate recycling. Using the computational framework developed, we show that this is challenging with current membrane materials, but that a well-designed hybrid process could still achieve significant reductions in overall energy consumption while being deployable with currently available technologies.