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Editorial

Modeling, Simulation, and Optimization of Membrane Processes

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From water desalination and gas purification to metal recovery and beyond, membrane separation has become integral to numerous industrial applications. Efficiency, cost-effectiveness, and sustainability of membrane processes can be enhanced through a fundamental analysis of complex transport phenomena and system-level behavior [1]. Modeling and simulation allow researchers to analyze their design configurations and operating conditions before spending time and money on large-scale testing. Optimization enables engineers to make the design most efficient while considering constraints.

The Special Issue of Separations, "Modeling, Simulation, and Optimization of Membrane Processes", aggregates eight articles with accomplished research that investigate cutting-edge advancements for membrane processes in fields such as energy, biomedical, water desalination, and wastewater treatment.

With advancements in 3D printing technology, the fabrication of novel complex membrane spacers for reverse osmosis desalination and ultrafiltration is possible [2]. Taking a concept from differential geometry, triply periodic minimal surfaces (TPMS) are 3D zero curvature repeating lattice-like structures with a maximized surface-to-volume ratios. Qiang Chen, Jiu Luo, and Yi Heng from Sun Yat-sen University investigated TPMS-based spacer designs for desalination by developing a mathematical mass and fluid transfer model [3]. Running CFD simulations, it was determined that TPMS modeled membrane spacers had less pressure drop across the membrane and higher permeate flux compared with commercially used spacers. The study showcases promising potential using mathematical shapes such as TPMS to improve production capacity for brackish water reverse osmosis desalination.

In another article from Sun Yat-sen university, Qingqing Yang, Yi Heng, Ying Jiang, and Jiu Luo utilized a multiscale modeling approach to analyze membrane characteristics using permeable and impermeable wall assumptions [4]. The two models differ such that the permeable model couples the fluid flow and mass transfer, while the impermeable wall model assumes zero permeation flux and applies constant concentration boundary condition on the membrane surface. It was determined that the impermeable wall approach reduced computational time with little effect on accuracy compared to the permeable wall models with some stipulations. However, local concentration polarization cannot be accurately predicted with the impermeable wall model.

An area of concern within wastewater treatment is copper, a heavy metal that has negative effects on biological health and the environment. R. Harharah and colleagues from King Khalid University, Saudi Arabia along with G. Abdalla from University of Khartoum, Sudan studied artificial copper wastewater RO separation on a benchtop skid [5]. Observed relationships and mathematical models of permeate flux and effective copper ion removal were developed considering operating pressure, feed temperature, feed concentration, and feed flowrate. Notably, permeate flux and ion removal increased with increase in operating pressure and feed temperature. Moreover, feed concentration inversely affected permeate flux and ion removal.

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Two of the articles concentrate on proposed novel reactors that implement membranes in their design. The addition of membranes in the Membrane Bioreactor-Membrane Distillation system (MBR-MD) and the Membrane Storage Reactor (MSR) demonstrates several advantages due to this implementation. While one article focuses on the environmental benefits of the proposed system and the other emphasizes the ways in which the reactor increases the intensity of products, both researched designs highlight the benefits of membrane technologies in reactors.

In Modeling and Life Cycle Assessment of a Membrane Bioreactor–Membrane Distillation Wastewater Treatment System for Potable Reuse, researchers from University of Nevada studied the Life Cycle Assessment (LCA) of a novel membrane bioreactor–membrane distillation (MBR-MD) system to analyze its environmental impact when treating water. With growing concerns over water scarcity, this novel system was compared to the most common wastewater treatment currently used, which is indirect potable reuse (IPR) [6]. The article concludes that the MBR-MD system has a significantly lower environmental impact than IPR when MD is operated with waste heat. However, the limitations are apparent as without waste heat being used, the MBR-MD system has a notably large environmental impact compared to the IPR system. The research demonstrated that the novel MBR-MD system has the potential to reduce a significant number of environmental impacts while addressing the issue of water scarcity effectively.

Another novel reactor was presented in the article, On Process Intensification through Membrane Storage Reactors, a joint work between University of California, Los Angeles and University of Southern California. The proposed design is a novel MSR that the researchers developed, simulated, and analyzed. The resulting data showed that the MSR would increase the yield of a desired species. The design implemented a semipermeable membrane boundary in between two physical areas in the reactor to increase the rate of production through dynamic operation [7]. Compared to the common steady state reactor currently being used in operations, the MSR proved to perform significantly better. The numerous advantages gained through the MSR process demonstrate the significance of improving process intensification technologies even at the industrial level.

Highlighted in this Special Issue is the use of specialized membranes that impact the energy production. Membrane research in the energy sector has used the concept of salinity gradient exchange (SGE), utilizing the chemical potential between waters of differing salinity levels [8]. The difference in salinity levels causes water to move across semipermeable membranes via the principles of osmosis where the energy is harvested using the pressurized water from the osmotic movement which can spin turbines to generate energy. This method is known as pressure retarded osmosis (PRO). Another method that capitalizes on the energy available from SGE is reverse electrodialysis (RED), in which membranes that selectively allow ions of fixed charges to pass known as ion exchange membranes (IEM). The electric potentials developed on the membranes can generate electric energy when applied to an external load.

In Modeling and Optimization of Membrane Process for Salinity Gradient Energy Production by Lianfa Song at Texas Tech University, the additional energy density was studied that can be achieved in PRO by manipulating the hydraulic pressures of the feed and draw sides of the semi-permeable membrane [9]. It was discovered that water flux can be increased by orders of magnitude by pumping the feed seawater across the membrane and exchanging some of the elevated pressure with incoming seawater, thereby allowing the draw side seawater to be at a higher pressure than the feed side fresh water. When compared to conventional PRO operation, the energy produced far surpasses the economical breakeven point, and shows a promising future for energy production.

Another article by the same group at Texas Tech University again addressed research in power production by SGE. In the publication, Accurate Determination of Electrical Potential on Ion Exchange Membranes in Reverse Electrodialysis, the performance of IEMs was studied via numerical solutions to the Nernst–Plank–Poisson (NPP) equations which best approximate the membrane potential in IEMs. In this paper, a boundary updating scheme developed in one of their previous papers is utilized to ensure that a true solution to the NPP equations and steady state is achieved [10]. The boundary updated NPP scheme is compared to the older, Teorell–Meyer–Siever (TMS) method classically used to assess IEMs. The work reported that the accuracy of their numerical method aligned with analytical methods to study membrane potentials. It also demonstrated the strength of the boundary updated NPP method at estimating membrane potentials when compared to the TMS method.

In the field of medical sciences, membranes have shown potential in the application of artificial lungs. Because of air pollution caused by rapid industrialization, globally, lung diseases have been a fatal challenge. Current technologies lack the ability to be sufficient for patients waiting for lung transplants or true replacements. Current solutions use polymeric hollow fiber membranes (HFMs) which rise concerns of fouling in their implementation [11]. In the paper Applying a Hydrophilic Modified Hollow Fiber Membrane to Reduce Fouling in Artificial Lungs, the authors studied the usage of new modified HFMs that can be used in the design of artificial lungs. Hydrophilic modifications of HFMs with polydopamine and peptoid allows them to be permanently resistant to protein fouling, a concern associated with older HFMs. The new peptoid-modified hollow fibers are biocompatible and show stable transport of oxygen in a bovine solution [12]. The research shows promise for implementation in respiratory support systems to treat patients with respiratory failure.

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