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Modeling of Mass Transfer through an Ion-Exchange Membrane in Lithium Recovery by Donnan Dialysis

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Lithium today has taken on growing importance with the rising global demand for its extraction, as it plays a significant role in the production of lithium-ion batteries for electric vehicles and renewable energy storage systems. Since primary resources are in finite supply, the need for efficient and sustainable methods of lithium recovery, particularly from waste streams, has grown in urgency. Apart from this, it is also important from an environmental perspective, as sustainable lithium recovery helps to restrict wastage, reduces the exploitation of natural resources, and helps in transition towards a more circular economy. One of the perspective techniques of lithium recovery is membrane crystallization using Donnan dialysis. In this process, a waste solution containing lithium cations and chloride anions is converted into lithium carbonate using anion-exchange membrane. Under the right conditions, lithium carbonate can be precipitated out from the solution. To optimize and better understand the process of lithium recovery, it is important to develop a mathematical model of Donnan dialysis ion transport mechanisms. This includes capturing the dynamic concentration changes within the both the ion-exchange membrane and the external bulk solutions. Mathematical modeling is an effective way of simulating the behavior of systems under varying operating conditions, reducing the need for extensive experimentation. In this context, the Nernst–Planck equation is the commonly used equation to describe the fluxes of charged species, with consideration of the combined effects of diffusion and migration in an electric field. When complemented by appropriate boundary conditions, electroneutrality constraints, and chemical equilibrium relations, the model provides a potent means for the analysis of ion selectivity, transport rates, and the formation potential of target compounds such as lithium carbonate. Additionally, such modeling facilitates process optimization and design and scale-up of efficient separation systems. During Donnan dialysis, the composition of the bulk solutions evolves over time as ions are selectively exchanged through the membrane. In open systems at atmospheric conditions, dissolved carbon dioxide equilibrates with the aqueous phase to form carbonate equilibria with species that include carbonic acid, and its dissociation products – bicarbonate and carbonate ions. These equilibria are sensitive to pH and ionic strength, and can affect both ion transport and the crystallization tendency of lithium carbonate. The model therefore includes dynamic changes in carbonate speciation in the bulk solutions in order to more accurately approximate real operating conditions.

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