Transport Modeling In Fumasep FAA-3-30 Membrane For Optimizing Direct Air Capture Systems

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Abstract

This study focuses on the time-dependent behavior of moisture and carbon diffusion within the Fumasep FAA-3-30 membrane, utilized in moisture swing Direct Air Capture (DAC) systems. Understanding the concentration distribution of the species within the membrane over time, water flux and also carbon flux is crucial for optimizing DAC systems, which are vital for mitigating carbon dioxide emissions. Enhanced membrane design can significantly contribute to more cost-effective and environmentally sustainable carbon capture solutions.

The problem setup involves using the Nernst-Planck Equations (NPE) interface from the Chemical Reaction Engineering Module in COMSOL Multiphysics® to model the diffusion, and migration of dissolved ionic species within the membrane over time. The simulations consider both constant and concentration-dependent diffusion coefficients for water, carbonate, and bicarbonate.

Results from the simulations with constant diffusion coefficients show that during the transition from dry to wet states, the moisture concentration within the membrane increases gradually, reaching a steady state after approximately three minutes. Conversely, the transition from wet to dry states reaches steady state after about four minutes. These findings indicate the time required for moisture concentration to equalize across the membrane.

Incorporating concentration-dependent diffusivity, derived from experimental data, revealed a non-linear concentration distribution of moisture, carbonate, and bicarbonate within the membrane. This non-linearity contrasts with the linear results obtained using constant diffusivity. The transition time for the membrane to saturate from a dry state is increased to about four and a half minutes, attributed to the lower range of the diffusion coefficient compared to the constant value of 4×10^{-12} m²/s.
Since there is no externally applied potential or closed electrical circuit, the net current density is approximately zero, maintaining electroneutrality. Although results show small values close to zero, these can be attributed to numerical simulation errors and minimized by refining the mesh sizes.

The study also identifies an electric field in the membrane resulting from the concentration gradient of ions, measured at around 16 mV. Additionally, the carbon flux, closely tied to the flux of carbonate and bicarbonate, is calculated to be approximately 135 μmol/(m²*s).

Future steps involve handling variable boundary conditions, including constant flux transitions from diffusion to convection and reactive flux scenarios. This will ensure a comprehensive understanding of the transport phenomena within the membrane.

Overall, this study provides valuable insights into the moisture diffusion behavior of the Fumasep FAA-3-30 membrane, which is essential for improving DAC system efficiency. The results highlight the significant impact of diffusion coefficients on transition times and underscore the

importance of accurate modeling for enhancing membrane performance. Future work will extend these findings by incorporating electric field effects, carbon fluxes, and refining boundary condition treatments, thereby contributing to the advancement of DAC technologies.

Reference

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