Proceedings of the 10th World Congress on Momentum, Heat and Mass Transfer (MHMT 2025)
Barcelona, Spain - April 08 - 10, 2025
DOI: 10.11159/ENFHT24.002

Estimation and Analysis of Transport Properties in Mixed-Matrix Membranes for Enhanced Gas Separation: An Integrated Experimental and Computational Study

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Abstract

Mixed-matrix membranes (MMMs) have emerged as a significant advancement in the field of gas separation technology. These innovative materials, which combine the benefits of organic polymers and inorganic fillers, have shown great potential in enhancing the efficiency of gas separation processes. This study aims to provide a comprehensive estimation of the transport properties of MMMs, with a particular focus on their permeability, diffusivity, solubility, and selectivity.

The transport properties of MMMs are primarily determined by three factors: the nature of the polymer matrix, the type of inorganic filler, and the interaction between the two. The polymer matrix provides the basic structure and mechanical stability of the membrane, while the inorganic filler enhances its separation performance. The interaction between the polymer and the filler, which can be tuned by modifying their chemical structures, plays a crucial role in determining the overall transport properties of the MMMs. To estimate these properties, we employ a combination of experimental measurements, empirical models, and computational simulations. Experimental measurements, such as gas permeation tests, provide direct information about the permeability, diffusivity, solubility, and selectivity of the MMMs. These tests are conducted under various conditions to investigate the effects of temperature, pressure, filler loading, and gas composition on the transport properties of the membranes.

On the other hand, computational simulations offer a microscopic view of the transport process. Using molecular dynamics simulations, we can observe the movement of gas molecules in the membrane and calculate their diffusion coefficients. Furthermore, quantum mechanical calculations allow us to evaluate the interaction energy between the gas molecules and the membrane materials, which is a key factor affecting the selectivity of the MMMs. By integrating the results from experiments and simulations, we can establish a comprehensive understanding of the transport properties of MMMs. This understanding enables us to identify the key factors that determine the performance of the membranes and to predict their behavior in different gas separation applications. Moreover, the estimation of transport properties provides valuable insights into the structure-property relationships in MMMs. It reveals how the structural features of the membranes, such as the size and distribution of the inorganic fillers, affect their transport properties. These insights can guide the design and optimization of MMMs for specific gas separation tasks.

In conclusion, this study presents a systematic approach to estimating the transport properties of mixed-matrix membranes used in gas separation. Results provide a solid foundation for the further development of MMMs, paving the way for their wide application in various industries.