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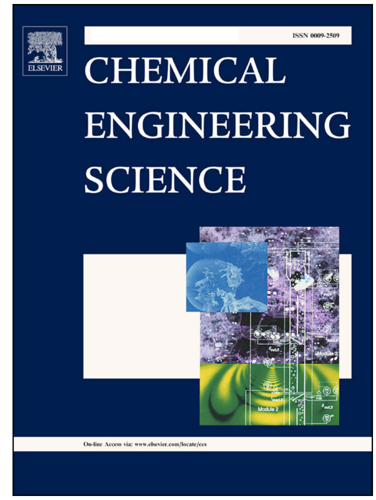

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The solute rejection of a nanoslit in osmosis

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Abstract

Two-dimensional nanoporous membranes have recently attracted great attention in osmosis-related applications due to their high water permeability and salt rejection. The size distribution of the pores on the membrane is closely related to these properties. Circular pores have been the main subject of research. Recently, it was found that the water permeability of a slit pore can be much higher than that of a circular pore, with the same salt rejection. Hence, it is necessary to discuss the osmotic flow through these pores at the nanoscale. In widely used models, two solute parameters are always used to quantify the ability to produce osmotic pressure and the probability of being rejected by the membrane. These are always assumed to have the same value and thus are both called *reflection coefficients.* However, this assumption is found to be inconsistent with the experimental results when describing osmosis on this scale. In this work, we discuss osmosis through a slit by making an analogy between the solute and the ideal gas molecules in the dilute solution. Expressions for the two *reflection coefficients* are derived based on the geometrical relationship between the solute and the slit. We find that the two coefficients increase with the size of the solute. Their values are not equal, as found in previous experiments. Extensive molecular dynamics (MD) simulations are performed and a good correlation between the simulation results and our predictions is found. This work may help to understand the osmotic flow through nanoscale pores and enable the design of highly efficient nanopores on membranes in osmosis-related applications.

Keywords

Osmotic flow; reflection coefficient; slit pore; physical model; molecular dynamics simulation

1. Introduction

Membrane-based separation processes are pervasive and crucial in osmosis-related applications(Wang et al., 2014a). High water permeability and salt rejection are generally required for efficient membranes (Werber et al., 2016). Recently, several two-dimensional materials used as novel membranes have earned much

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