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Solvent nanofiltration through polybenzimidazole membranes: unravelling the role of pore size from molecular simulations

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ABSTRACT

There has been considerable interest in the use of polymer membranes for solvent nanofiltration. While the pore size of nanofiltration membranes is generally known to be within 0.5-2 nm, the precise control of pore size and quantitative understanding of the role of pore size are experimentally challenging. By molecular simulations, in this study, we investigate solvent nanofiltration through polybenzimidazole (PBI) membranes with different pore sizes. Five PBI model membranes are constructed and pretreated by methanol, with the mean pore size (MPZ) ranging from 3.53 to 6.38 Å. When the MPZ increases, large pores are more populated and connected in the membrane. It is revealed that methanol permeation is governed by the presence and interconnectivity of large pores. For the membrane with a MPZ of 6.38 Å, the permeation of methanol and water is simulated. Compared with methanol, water permeation is faster but slowed down at a later stage due to the membrane compression. The rejection of a model solute, glucose, is found to be 100%. This simulation study highlights the crucial role of pore size, as well as pretreatment, in solvent permeation, and would facilitate the development of new membranes for high-performance solvent nanofiltration.

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