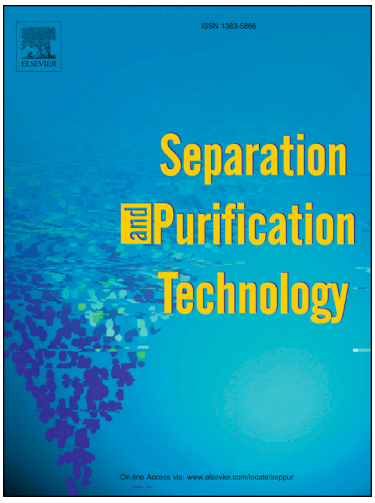

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Efficient Separation of Helium from Methane using MOF Membranes

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Abstract

Traditional separation methods of helium recovery are energy intensive and economically disadvantageous. Considering the potential deficit of helium, it is very important to develop efficient technologies for helium recovery from natural gas sources. Metal organic frameworks (MOFs) have emerged as strong alternatives to traditional membrane materials due to their wide range of pore sizes, permanent porosities, and high surface areas. Only a small number of MOF membranes has been fabricated and experimentally tested for He/CH_4 separations. In this study, we performed the first large-scale computational study to predict He/CH_4 separation performances of various MOF membranes. First, we compared predictions of our molecular simulations with the experimentally available data for He permeability of several MOF membranes. Motivated from the good agreement between experiments and simulations, we examined 139 different MOF membranes for He/CH_4 separation. Selectivity and permeability of the MOF membranes were compared with those of traditional polymer and zeolite membranes. A significant number of MOF membranes was identified to exceed the Robeson's upper bound due to their high gas selectivities and permeabilities. We also compared ideal and mixture selectivities of MOF membranes performing molecular simulations both for single-component gases, He and CH_4, and binary gas mixtures of He/CH_4. Results showed that selectivities and permeabilities of MOF membranes calculated using the single-component gas data can significantly overestimate the ones calculated using the mixture data. Results of this study will be useful to guide the experiments for selecting the most promising MOF membranes for efficient He/CH_4 separations.

Keywords: metal organic frameworks, gas separation, membrane, selectivity, permeability, helium recovery

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