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A Mass Transfer Model for Pervaporation Separation Processes in Mixed Matrix Membrane

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Extended Abstract

Pervaporation, a membrane-based process, is considered to be a promising technique for the separation of organic compounds from aqueous solutions [1]. Different types of polymeric membranes have been used for this process due to their wide range of component separation properties, easy fabrication and low membrane fabrication cost per unit membrane area [1]. However, these types of membranes are suffering from the trade-off between permeability and selectivity. There are many studies which have investigated the incorporation of the nanoporous particles such as zeolites [2], metal organic frameworks (MOFs) [3], carbon nanotubes (CNTs) [4], silicalites [5] and activated carbon (AC) nanoparticles [1] into the matrix of polymeric membranes to improve their performance. It has been reported that mixed matrix membranes have higher permeability, higher selectivity or both in comparison with neat membranes of the same polymer type. In order to have a better understanding on the effects of the particles in the matrix of the membrane and the mixed matrix membrane performance behaviour, a mathematical model is necessary. Moreover, a reliable mathematical model is needed for the optimization of the process at an industrial scale. The majority of the models which have been reported in the literature considered the application of mixed matrix membranes for gas separation processes and, to the best of our knowledge, this investigation is one of the first studies to model these types of membranes for pervaporation applications.

In this study, a novel mass transfer model for pervaporation separation through a flat mixed matrix membrane (MMM) has been developed to predict the effective permeability of the permeating components. A 3D structure of a mixed matrix membrane with randomly dispersed particles for different volume fractions has been considered and solved by the finite difference method. In addition, the effect of permeability ratio of the dispersed phase to the continuous phase, the particle size, the particle shape and the membrane thickness has been investigated. The Fickian diffusion equation was used to calculate the concentration profile of the components through the membrane. Moreover, it was assumed that there is an ideal interface between the dispersed and the continuous phase.

Figure 1 presents the effective permeability of the mixed matrix membrane as a function of the relative permeability (ratio of the dispersed phase over the continuous phase) and the particle loading. The effective permeability of the mixed matrix increases with an increase in the particle loading when the particles are more permeable than the polymer. The increase is more pronounced for a higher relative permeability. When the permeability of the dispersed phase is smaller than the permeability of the continuous phase, the effective permeability decreases and the mixed matrix membrane acts more like a barrier material.

This investigation also considered different shapes of particles such as cubical, spherical and cylindrical (in vertical and horizontal orientation) on the effective permeability of the mixed matrix membrane. Simulations showed that the membrane performance is only a function of the particle shape at higher particle concentrations, i.e. for volume fractions greater than 40% which is far beyond the typical range of particle loading in mixed matrix membranes.



Fig. 1: Effect of the ratio of the permeability of the dispersed phase permeability to the continuous phase on the membrane effective permeability.

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