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Transport properties of thermally rearranged polymeric membranes

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ABSTRACT

Rigid polymer membranes are recently regarded as state of the art materials for gas separation processes, due to their high permeability and selectivity [1]. Among them, thermally rearranged polybenzoxazole (TR-PBO) has been showing not only outstanding mechanical and chemical stability but also high permeability that surpass the limits of conventional polymers [2-4]. In this study, we analyzed the transport properties of the rigid thermally rearranged polybenzoxazoles (TR-PBOs) of single gases (CO_2 and N_2) and binary gas mixture of CO_2 and N_2 at a corresponding trans-membrane pressure difference of five bar. GCMC simulation for solubility and calculation of diffusivity were performed with each 3D model. The results revealed that the CO_2 permeability calculated under the mixed-gas condition remained the same as the single gas CO_2 permeability, while that of N_2 decreased, thus leading to a favored increase in selectivity. Consequently, we could integrate our simulation results with the experimental findings already reported in the literature yielding insightful indications and finally establish the role of molecular structure on their perm-selective behavior. rigid polymer membranes.

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