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Thin film composite membranes based on a polymer of intrinsic microporosity derived from Tröger's base: A combined experimental and computational investigation of the role of residual casting solvent

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Abstract

Composite membranes were developed for gas separation applications, both as flat-sheets and hollow fibres, using a Polymer of Intrinsic Microporosity, composed of Tröger's base, TB, and of ethanoanthracene (PIM-EA(H_2)-TB) as the selective layer. The crucial role of the solvent, dichloromethane and chloroform, used in membrane preparation on the transport properties was evaluated by both thermogravimetric analysis and permeation tests on PIM-EA(H_2)-TB dense self-supported films. Molecular modelling, reproducing the experimental conditions in presence of the two different solvents, was performed to investigate the role of the solvent on the morphological and transport properties of the PIM polymer. The strong interaction of the polymer matrix with chloroform reduces gas permeability due to the partial saturation of the sorption sites and the competition between solvent and permeating gas molecules. Consequently, dichloromethane was chosen as suitable solvent in composite membrane preparation also for its good compatibility with PAN. PAN-based hollow fibres were prepared according to phase inversion method and used as porous supports. They were functionalised by partial conversion of the nitrile groups into carboxyl groups to improve compatibility with the active PIM layer. Controlled temperature and humidity conditions during the coating process reduced the presence of micropores on the membrane surface, favouring the formation of a dense layer on the hollow fibre porous support. Composite PIM-EA(H_2)-TB membranes were successfully developed having selectivity similar to the dense membranes for different gas pairs.