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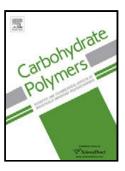
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ACCEPTED MANUSCRIPT

Chitosan-polytetrafluoroethylene composite membranes for separation of methanol and toluene by pervaporation

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Research Highlights

- Facile separation of methanol/toluene azeotrope using a novel TEOS crossed composite chitosan/PTFE membrane.
- TEOS cross-linking improved separation factor and thermal stability.
- A combination of Molecular Dynamics and CFD simulations enabled performance prediction of commercial pervaporation systems.
- High potential for membrane scale up owing to its composite structure.

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Abstract

Present work reports the synthesis of a novel Chitosan-Polytetrafluoroethylene composite membrane with solvent resistant property for efficient separation of methanol/toluene mixture by pervaporation. The composite was crossed with tetraethyl orthosilicate (TEOS) to prevent or reduce membrane swelling and improve the separation factor. The synthesized membranes were characterized by SEM, FTIR and DSC analysis. Molecular dynamics (MD) simulation and computational fluid dynamics were coupled to predict the structural and diffusive properties besides concentration profile inside the membrane. Diffusion coefficients of methanol and toluene were found to be 1.7 x10⁻⁹ and 1.8 x 10⁻¹² m²/s, respectively. The effect of crosslinking on process parameters such as flux and separation factor was analyzed. The study

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