Desalination and Water Treatment
www.deswater.com

doi: 10.5004/dwt.2020.26214

203 (2020) 58–69
November

Effect of $CaCl_2$ addition on crystal structure and separation performance of PVDF membranes: an experimental and molecular simulation study

Yue Song[a], Jiacong Li[a], Guorong Xu[b], Ming Zhang[a,*], Hai Xin[a], Zihan Liu[a], Xintao Zuo[a], Wenyuan Fan[a]

[a]*School of Chemistry and Chemical Engineering, Tianjin Key Laboratory of Organic Solar Cells and Photochemical Conversion, Tianjin University of Technology, Tianjin 300384, China, Tel. +86 22 6021 4259; emails: zm2404@tjut.edu.cn (M. Zhang), 15822763588@163.com (Y. Song), ljc9433@163.com (J. Li), xin13821765171@163.com (H. Xin), lzhan424@163.com (Z. Liu), xintaozuo@126.com(X. Zuo), wyfan@tjut.edu.cn (W. Fan)*

[b]*The Institute of Seawater Desalination and Multipurpose Utilization, Ministry of Nature Resources (MNR), Tianjin 300192, China, Tel. +86 22 8789 6336; email: laxgr@aliyun.com (G. Xu)*

Received 4 November 2019; Accepted 6 June 2020

ABSTRACT

The inorganic salts addition can affect the interactions among the polymer chains and further influence the membrane structure. In this work, the effects of calcium chloride ($CaCl_2$) on the crystal structure and separation performance of poly(vinylidene fluoride) (PVDF) membranes were studied. The influence of $CaCl_2$ addition with varying concentrations (0–3 wt.%) was investigated by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and molecular dynamic (MD) simulations. XRD and FTIR characterizations indicated that $CaCl_2$ could induce the transformation of PVDF crystal structure from α to β, which was further confirmed by molecular dynamic simulation. The MD simulation results revealed that the interaction between Ca^{2+} and F atom distorted the dihedral angle of PVDF chains, inducing the crystal structure transforming partially. SEM characterization indicated that the finger-like voids became longer and broader with increasing amount of $CaCl_2$ addition. The membrane consisting of 0.7 wt.% $CaCl_2$ exhibited the best performance with bovine serum solution rejection of 84.7% and water permeability of 203.6 L m^{-2} h^{-1} bar^{-1}.

Keywords: Calcium chloride; PVDF membrane; Crystal form transform; Molecular dynamic simulation; Mechanism

* Corresponding author.