Received: 3 July 2020 | Revised: 27 August 2020 | Accepted: 15 September 2020

DOI: 10.1002/pen.25547

RESEARCH ARTICLE

POLYMER ENGINEERING AND SCIENCE WILEY

An atomistic simulation towards molecular design of silica polymorphs nanoparticles in polysulfone based mixed matrix membranes for CO_2/CH_4 gas separation

Serene Sow Mun Lock[1] | **Kok Keong Lau**[1] | **Norwahyu Jusoh**[1] | **Azmi Mohd Shariff**[1] | **Chin Heng Gan**[2] | **Chung Loong Yiin**[3]

[1]CO2 Research Center (CO2RES), Department of Chemical Engineering, Universiti Teknologi PETRONAS, Seri Iskandar, Perak, Malaysia

[2]Department of Civil Engineering, Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Jalan Sungai Long, Bandar Sungai Long, Cheras, Kajang, Selangor, Malaysia

[3]Department of Chemical Engineering and Energy Sustainability, Faculty of Engineering, Universiti Malaysia Sarawak (UNIMAS), Kota Samarahan, Sarawak, Malaysia

Correspondence
Kok Keong Lau, CO2 Research Center (CO2RES), Department of Chemical Engineering, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Malaysia.
Email: laukokkeong@utp.edu.my

Funding information
Murata Science Foundation, Grant/Award Number: 18 MP04

Abstract

Incorporation of inorganic fillers into Polysulfone (PSF) to constitute mixed matrix membranes (MMMs) has become a viable solution to prevail over limitations of the pristine materials in natural gas sweetening process. Nevertheless, preparation of MMMs without defects and empirical investigation of membrane that exhibits characteristic of improved CO_2/CH_4 separation performance at experimental scale are difficult that require prior knowledge on compatibility between the filler and polymer. A computational framework has been conducted to construct validated PSF based MMMs using silica (SiO_2) as inorganic fillers. It is known that nanosized SiO_2 can coexist in varying polymorph configurations (ie, α-Quartz, α-Cristobalite, α-Tridymite) but molecular simulation study of SiO_2 polymorphs to form MMMs is limited. Therefore, this work is a pioneering study to elucidate feasibility in facile utilization of polymorphs to improve gas separation performance of MMMs. Physical properties and gas transport behavior of the simulated PSF based MMMs with different SiO_2 polymorphs and loadings have been elucidated. The optimal MMM has been found to be PSF/25 wt% α-Cristobalite at 55°C. The success in molecular simulation has shed light on how computational tools can provide understandings at molecular level to elucidate compatibility between varying pristine materials to MMMs for natural gas processing.

KEYWORDS

CO_2/CH_4 separation, membrane, molecular simulation, polysulfone, α-Cristobalite, α-Quartz, α-Tridymite

1 | INTRODUCTION

Carbon dioxide (CO_2) capture from natural gas is essential to comply with methane (CH_4) product specification while simultaneously mitigating greenhouse gas environmental effect.[1] Glassy polymeric membrane typically Polysulfone (PSF) dominates membrane gas separation in industry attributed to its economical production cost and ease of replication for huge scale fabrication.[2] However, the performance of PSF polymeric membrane in CO_2/CH_4 separation encounters constraint in trade-off between permeability (high CO_2 gas transport to accommodate application with big feed capacity and high CO_2 impurities) and selectivity (preference to allow transport of CO_2 while retaining CH_4 in another stream).[3] Development of mixed matrix membranes (MMMs) through

 © 2020 Society of Plastics Engineers