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A systematic review of the molecular simulation of hybrid membranes for performance enhancements and contaminant removals

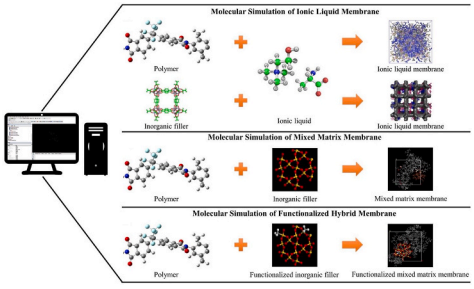
Cia Yin Yee [a], Lam Ghai Lim [b], Serene Sow Mun Lock [a,*], Norwahyu Jusoh [a], Chung Loong Yiin [c,d], Bridgid Lai Fui Chin [e,f], Yi Herng Chan [g], Adrian Chun Minh Loy [h], Muhammad Mubashir [i]

[a] CO_2 Research Center (CO2RES), Department of Chemical Engineering, Universiti Teknologi PETRONAS, 32610, Seri Iskandar, Perak, Malaysia
[b] School of Engineering, Monash University Malaysia, 47500, Bandar Sunway, Selangor, Malaysia
[c] Department of Chemical Engineering and Energy Sustainability, Faculty of Engineering, Universiti Malaysia Sarawak (UNIMAS), Kota Samarahan, 94300, Malaysia
[d] Institute of Sustainable and Renewable Energy (ISuRE), Universiti Malaysia Sarawak (UNIMAS), 94300, Kota Samarahan, Sarawak, Malaysia
[e] Department of Chemical and Energy Engineering, Faculty of Engineering and Science, Curtin University Malaysia, CDT 250, 98009, Miri Sarawak, Malaysia
[f] Energy and Environment Research Cluster, Faculty of Engineering and Science, Curtin University Malaysia, CDT 250, 98009, Miri Sarawak, Malaysia
[g] PETRONAS Research Sdn. Bhd. (PRSB), Lot 3288 & 3289, Off Jalan Ayer Itam, Kawasan Institusi Bangi, 43000, Kajang, Selangor, Malaysia
[h] Department of Chemical Engineering, Monash University, Clayton, VIC, 3800, Australia
[i] Physical Science and Engineering Division, Advanced Membranes and Porous Materials Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

HIGHLIGHTS

- Fundamentals of molecular simulation are reviewed and related to application in hybrid membranes.
- Insight into molecular structural properties of hybrid membranes is presented.
- Simulated transport performance from published literature and mechanism of hybrid membranes are provided.
- Limitation in molecular simulation for membrane separation is discussed.
- Future outlook for molecular simulation of membrane separation is recommended.

GRAPHICAL ABSTRACT



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ABSTRACT

Number of research on molecular simulation and design has emerged recently but there is currently a lack of review to present these studies in an organized manner to highlight the advances and feasibility. This paper aims to review the development, structural, physical properties and separation performance of hybrid membranes using molecular simulation approach. The hybrid membranes under review include ionic liquid membrane, mixed matrix membrane, and functionalized hybrid membrane for understanding of the transport mechanism of molecules through the different structures. The understanding of molecular interactions, and alteration of pore sizes and transport channels at atomistic level post incorporation of different components in hybrid membranes posing impact to the selective transport of desired molecules are also covered. Incorporation of molecular simulation of hybrid membrane in related fields such as carbon dioxide (CO_2) removal, wastewater treatment,

* Corresponding author. Department of Chemical Engineering, Universiti Teknologi PETRONAS, Bandar Seri Iskandar, 31750, Tronoh, Perak, Malaysia.
E-mail address: sowmun.lock@utp.edu.my (S.S.M. Lock).

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and desalination are also reviewed. Despite the limitations of current molecular simulation methodologies, i.e., not being able to simulate the membrane operation at the actual macroscale in processing plants, it is still able to demonstrate promising results in capturing molecule behaviours of penetrants and membranes at full atomic details with acceptable separation performance accuracy. From the review, it was found that the best performing ionic liquid membrane, mixed matrix membrane and functionalized hybrid membrane can enhance the performance of pristine membrane by 4 folds, 2.9 folds and 3.3 folds, respectively. The future prospects of molecular simulation in hybrid membranes are also presented. This review could provide understanding to the current advancement of molecular simulation approach in hybrid membranes separation. This could also provide a guideline to apply molecular simulation in the related sectors.

1. Introduction

In recent years, hybrid membranes have rapidly emerged as a promising technology to circumvent limitation in polymeric membranes for separation process. Hybrid membranes have the advantage of combining two material classes that can potentially modify the resultant structure, which outperform conventional membranes. High selectivity and permeability that are superior to the Robeson plot have been achieved, along with durable and optimized functions suited for specific applications. Different materials have been studied and reviewed for this purpose, but they are mostly limited to state of art research using experimental approach. Recently, computational chemistry has emerged as an indispensable tool to design new generation hybrid membranes with improved separation performance. This enables minimization of intervention from costly and time-consuming experimental method while providing insights at the atomic level, which is challenging or impossible to be measured using laboratory instruments.

Molecular simulation is used to resolve the undiscovered aspects of a system, often much cheaper compared to experiments (Mollahosseini and Abdelrasoul, 2021). Other advantages include the feasibility of designing different simulation perspectives via manipulation of computational approaches. In addition, simulation assists in testing conditions that are almost impossible at laboratory scales and reduces the handling of hazardous materials.

Investigation and analysis of the structural, physicochemical and transport behaviour of molecules through varying types of materials with different system parameters can be accessible at the molecular or atomistic level. The study variables may comprise glass transition temperature (T_g), pore size, fractional free volume, molecular interaction, X-ray diffraction, solubility, sorption and diffusion mechanisms (Dehghani et al., 2017). This has frequently found its application in estimation and calculation of various separation applications, which include gas purification, biomedical engineering and wastewater treatment (Ebro et al., 2013; Hollingsworth and Dror, 2018; An et al., 2019).

Alternatively, membrane system has an emerging role as a recognized eco-friendly separation process due to its low energy consumptions in post-combustion carbon dioxide (CO_2) capture and storage, natural gas sweetening, tertiary-level enhanced oil recovery, dehumidification, separation of acid gases, e.g., hydrogen sulphide (H_2S), sewage treatment, desalination, and pharmaceutical (Brunetti et al., 2015; Le and Nunes, 2016; Vara et al., 2020). In separation process utilizing membrane technology, membrane functions as a selective barrier to allow permeation of one selective permeate while retaining other components (Zolghadr et al., 2021; Manikandan et al., 2022). Permeability and selectivity are critical factors that affect the transport performance of membranes. Permeability of porous membrane is affected by the permeate molecule size in which larger components have lower diffusion coefficient and vice versa. On the other hand, permeability of non-porous membrane is influenced by the sorption of penetrant molecules into the membrane, its diffusion through the membrane, and desorption at the downstream of the membrane, which is known as the solution-diffusion mechanism (Freeman, 1999). Non-porous dense film membranes transport solute through the pressure difference, concentration, or electric-field gradients on upstream and downstream sides of the membrane (Rackley, 2017). Membrane selectivity is the ratio of permeability of the relevant permeate and retentate passing through the membrane (Zolghadr et al., 2021).

The three core membrane materials used in various industries for separation purposes are organic (polymeric), inorganic (graphene, carbon, zeolite, ceramic, metal, etc) and ionic liquid (He et al., 2018). Polymeric membrane is robust and easy to fabricate, but it has disadvantages of lower performance due to its inherent permeability-selectivity trade-off (Wu et al., 2020) (Freeman, 1999; Wong and Jawad, 2019). Substantial efforts have been ongoing to improve permeability and selectivity of organic membranes to increase its commercial competitiveness. On the other hand, inorganic membranes have excellent permeability, but their fabrication costs are generally higher (Jusoh et al., 2016). Ionic liquids (ILs) are salts made through association of large organic cations with a wide variety of anions, which offer high flexibility in designing new generation advanced materials for contaminant removal (Swati et al., 2021). ILs also inherit downsides, which include high viscosity, high cost, toxicity in abundant amount, which hinder their further expansion in industrial application.

A combination of the aforementioned materials is known as hybrid membrane. Hybrid membranes, a breakthrough of membrane technology, integrate the advantages of polymeric or inorganic or ionic liquid materials together (Jusoh et al., 2016). Hybrid membrane may be a solution to improve and modify the intrinsic property of the pristine material in a less costly manner and to be engineered to a specific use. Some of the crucial parameters for designing an efficient hybrid membrane include the selection of materials for the polymer, inorganic filler and ionic liquid, the composition of the selected materials, and operating conditions (Singh, 2005; Liguori and Wilcox, 2018; Gokulakrishnan et al., 2021).

Acting as an experiment guide, molecular simulation tool can be used to provide atomistic understanding and characterization of the tailor-made combination of membrane materials, its individual polymer, filler and ionic liquid (Keskin and Alsoy Altinkaya, 2019). Currently, comprehensive study of molecular structure of hybrid membranes and their separation mechanism is limited. This may be due to the reason that hybrid membranes are still mainly applied in laboratory settings and have yet to be widely applied in industry (Golzar et al., 2017a). The excellent separation performance reported in laboratory studies may pave the way for hybrid membranes to expand its use in industry but further elucidation from molecular simulation is required.

In this paper, a systematic review of the recent advances in membrane development for gas separation, water desalination, and wastewater treatment are presented. This includes the basic principles of different membrane processes using molecular simulation, such as ionic liquid membrane (ILM), mixed matrix membrane (MMM), and functionalized hybrid membrane (FHM). Subsequently, recent studies on membrane advances in various applications are reviewed. Lastly, future perspectives on the development of membrane separation using molecular simulation technique are provided.