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Development of hybrid models for prediction of gas permeation through FS/POSS/PDMS nanocomposite membranes

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ABSTRACT

The present paper aims to use intelligent methods for prediction of gas permeation in binary-filler nanocomposite membranes containing fumed silica (FS) and octa-trimethylsiloxy polyhedral oligomeric silsesquioxane (POSS) nanoparticles incorporated within a polymer matrix of polydimethylsiloxane (PDMS). Two reliable and rigorous hybrid models, i.e., differential evolution-adaptive neuro-fuzzy inference system (DE-ANFIS) and coupled simulated annealing-least square support vector machine (CSA-LSSVM) were developed in order to predict pure gas permeability of including H_2, CH_4, CO_2, and C_3H_8 through the nanocomposite membranes. The coupled simulated annealing (CSA) optimization algorithm was also used for tuning of the model parameters. The impacts of several key parameters such as pressure, FS nanoparticles loading as well as the kinetic diameter of gases on permeation were investigated. The experimental data were randomly divided into two main groups, namely training (70%) and testing (30%) sets. The results of the study suggested that DE-ANFIS model is a more robust and accurate model than the CSA-LSSVM with the R^2 values of 0.9981 and 0.9689, respectively.

Introduction

Among the currently-available technologies being used for gas and/or liquid separation, membrane separation has gained much attention recently [1–3] due to its applications in a variety of processes such as gas and petrochemical industries, purification of oxygen and nitrogen from the air, CO_2 capture and elimination of H_2S from natural gas, hydrogen production, and removing of undesired organic

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aerosol mist from air [4,5]. By rendering a feasible process with lower capital and utility costs, the membrane-based separation technology has found to be the promising alternative solution for many conventional methods which consume much energy for separation [6]. The recently increasing trend in using membrane technology in different fields has provided the motivation for many researchers to delve into the development of quick and state-of-the-art techniques and strategies to find the optimal performance of the membrane-based separation systems [7].

Membrane technology has been recognized as a practical solution for the recollection of heavier and valuable hydrocarbons from a light gas mixture system unlike its expensive conventional counterparts such as cryogenic distillation [8]. Polymer-based membranes which are fabricated from an organic selective material such as poly(dimethylsiloxane) (PDMS) or poly(1-trimethylsilyl-1-propyne) (PTMSP) have been suggested for this aim which provide a considerable selectivity to the heavier hydrocarbons (C_{3+}), and result in the separation of heavier hydrocarbons from the light gas mixtures such as CH_4, H_2, O_2, etc. In the previous studies, PDMS has shown to be selective membrane for removal and purification of H_2 in which high selectivity has been obtained due to its repeating unit [9–13]. PDMS nanocomposites, in particular, have shown to be a great choice for this type of membranes because of their several advantageous features such as high thermo-oxidative stability, large flexibility, lower glass transition temperature (T_g) and surface free energy, and being chemically less reactive compared to the other alternatives [14]. Despite the great chain flexibility and their good resistance with thermal degradation and also presenting thermo-oxidation in a larger range of temperature, the neat PDMS-based membranes suffer from low and non-optimal performance, thus may not be appropriate for industrial applications [15]. This issue can be tackled by incorporating some inorganic materials to the polymer structure by either polymerization or physical blending. Fumed Silica (FS) has been widely used for this aim and has been demonstrated to be a promising option for improving PDMS properties and characteristics for general applications especially in rubber industry [16,17]. Membranes with different combinations of nanocomposites have also been of interest with enhanced separation properties and higher resistance against thermal degradation [18–21]. Notably, the addition of polyhedral oligomeric silsesquioxane (POSS) to FS material results in improving several main properties of nanocomposite membranes such as better mechanical, thermal and operational performance, along with a more facile processing [12,22].

Experimental studies and pilot plant tests are extensively used to investigate novel design in membrane technology; however, these studies are time-consuming, expensive, and inefficient thus new approaches should be sought for alternative [23]. Apart from this, several features of the gas separation process by membranes, such as non-linearity of the underlying system equations with multiple variables, fairly large delay time, severe coupling of the equations and large uncertainty are among of other issues that make the experimental studies and conventional methods more challenging [24]. Furthermore, adopting conventional approaches for modeling and design of membranes are also problematic due to four reasons: (i) only a little knowledge is known about the governing mechanisms even for some of the most established membrane processes, i.e. reactive membranes; (ii) The important role of intermediate reactions cannot be neglected in many reactive systems; (iii) traditional methods are not generally capable of capturing some of the influential hidden variables and factors such as adsorbed surface components; (iv) difficulties with specifying the rate determining step, since it may be a function of operating conditions [7].

Artificial intelligence (AI) approaches have found to be a promising alternative to the conventional methods as they have a high capability of learning and modifying complicated processes [25]. Specifically, in most cases wherein our knowledge of the physical and chemical factors are scant, and the underlying variables may not be easily correlated without rendering an appreciable amount of errors, AI is an excellent choice of interest. Moreover, AI may be the best option for modeling and unraveling the practical problems especially those processes with non-linear systems [26]. A quick look at the literature reveals that AI has been used successfully for designing and developing membranes by a number of researchers [9,11]. Rezakazemi et al. [27] employed Artificial Neural Network (ANN) for predicting the gas sorption (H_2, CH_4, and CO_2) in a membrane with a combination of zeolite 4A nanoparticles evenly dispersed into a matrix of PDMS. Using a mathematical model which was able to sufficiently estimate the specific surface area of a glassy polyimide membrane, Peer et al. [28] numerically simulated the separation of H_2/CO mixture and validated with the experimental data collected from the literature. Also, an ANN model was developed and the GS behavior of the membrane was investigated. Recently, Dashti et al. [9] investigated the single sorption of C_3H_8, H_2, CH_4, and CO_2 within an H_2-selective nanocomposite membrane by developing several artificial models including MLP-ANN, ANFIS, GA-ANFIS, GP, and CMIS. The effects of critical temperature, upstream pressure, and nanoparticles loading were examined. The results of the study demonstrated the superiority of CMIS model over others in terms of simplicity, high accuracy, and generality.

In the light of the brief literature review conducted here, the motivation of the present study was formed. The paper aims to investigate the separation of a single gas by a novel membrane design comprising FS and POSS nanoparticles into a polymer matrix of PDMS by developing novel and easily implemented intelligent models, namely least square support vector machine (CSA-LSSVM) and differential evolution-adaptive neuro-fuzzy inference system (DE-ANFIS). The developed LSSVM model is trained and optimized by using CSA and the minimization of a cost function of Mean Squared Error (MSE). For the DE-ANFIS model, DE is coupled with the ANFIS to optimize the ANFIS variables and also making a trade-off between the complexity of the implementation of the model and its generality. The reliability of the developed models is also confirmed by adopting a number of statistical and graphical representations.

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