Journal of Membrane Science 687 (2023) 122025

Contents lists available at ScienceDirect

Journal of Membrane Science

journal homepage: www.elsevier.com/locate/memsci

Predicting the performance of organic solvent reverse osmosis membranes using artificial neural network and principal component analysis by considering solvent–solvent and solvent–membrane affinities

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ARTICLE INFO

Keywords:
Hansen solubility parameter
Polymer membrane
OSRO performance prediction
Solvent separation
Sustainability

ABSTRACT

The prediction of organic solvent reverse osmosis (OSRO) performance is challenging because of the numerous variables influencing the process. Therefore, applying a machine learning model, such as an artificial neural network (ANN), instead of physics-based modeling is helpful because it can consider many variables and learn patterns to generate a prediction. However, limited experimental data, along with the numerous variables that influence the OSRO process, considerably hamper the proper training of an ANN. Moreover, the affinities between membranes and solvents and between solvents play an important role in OSRO performance. Thus, new variables should be considered for appropriately training the ANN. However, this consideration further increases the number of variables. Herein, we proposed new variables that considered all three components of the Hansen solubility parameters for the membranes and the involved solvents to represent their interactions. Principal component analysis (PCA) was performed to simplify the information from multiple variables and extract only the main information to evaluate the importance of the input variables. The results from PCA were used as fundamental inputs in constructing the ANN model. Additionally, some OSRO-relevant variables, including applied pressure, solvent fraction, and solubility parameters, were used to train the multilayer perceptron ANN, and its structure was optimized using a genetic algorithm. To the best of our knowledge, this is the first time that the OSRO performance is predicted using machine learning. The average absolute relative deviation values between the model-calculated and experimental data were 6.81% and 1.84% for flux and rejection, respectively. Our findings demonstrated that the proposed new variables significantly improved the OSRO predictions.

1. Introduction

Organic solvents are essential chemicals that are widely used in various industries, including pharmaceuticals [1,2], batteries and fuel cells [3], cosmetics and beauty [4], paint and coatings [5], food [6] and agriculture, petrochemicals [7], and oil [1]. However, the separation of organic liquid mixtures is still largely performed using energy-intensive thermal processes, such as distillation and evaporation, which constitute approximately 10%–15% of global energy consumption [8]. Thus, organic solvent nanofiltration (OSN) and organic solvent reverse osmosis (OSRO) using solvent-resistant membranes have emerged as energy-efficient alternatives to separation processes employed for organic solvents [8]. They also have several advantages, such as mechanical flexibility and easy scale-up. OSN is mainly used to separate

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https://doi.org/10.1016/j.memsci.2023.122025
Received 26 June 2023; Received in revised form 18 August 2023; Accepted 22 August 2023
Available online 23 August 2023
0376-7388/