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Multiscale computational modeling of organic compounds separation using microporous membranes

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ABSTRACT

Computational modeling and numerical simulation of separation processes have been carried out in this work. A computational model is developed and numerically solved to calculate and obtain the concentration of a liquid solution in a pervaporation membrane process. The model considers basic conservation equations for the solution of water/alcohol in a membrane separation process. The governing equations are then solved and interpreted using computational fluid dynamics approach in order to optimize and design the process of interest. The results of computational simulations indicate that the model is well developed and can predict the performance of separation process with high accuracy.

Keywords: Computational modeling; Numerical simulation; Purification; Alcohol; Water

1. Introduction

Development of theoretical models for prediction, design, and optimization of chemical processes is of great importance [1–4]. Among various chemical processes, separation processes play a crucial role in chemical industry and optimization of chemical processes can improve the efficiency of the whole process significantly [5–12]. Theoretical modeling and simulation of separation processes can be a great tool in order to better understand the process, and can design the process at both pilot and industrial scale [13–16]. There are different types of models developed for process modeling and simulation available in literature including artificial neural network models, mechanistic models, and semi-mechanistic models. Application of each modeling approach depends on the process and different phases available in the process [12,17–22]. Recently computational fluid dynamics approach has attracted much attention in process modeling and simulation [23–28]. Some authors have used different modeling approaches for simulation of chemical processes [29–37].

In this study, a computational model is developed for simulation of a chemical process used for separation and purification of water/alcohol solutions. The model is developed based on conservation equations and the computational fluid dynamic approach is used for numerical simulation of the process.

2. Computational model of the process

For the development of the computational model, a geometry of process is drawn which is shown in Fig. 1. As seen, the process involves separation of a solution of water/alcohol by a membrane which divides the two solutions. The membrane acts as a separation medium for two phases and the separation occurs during the membrane module.

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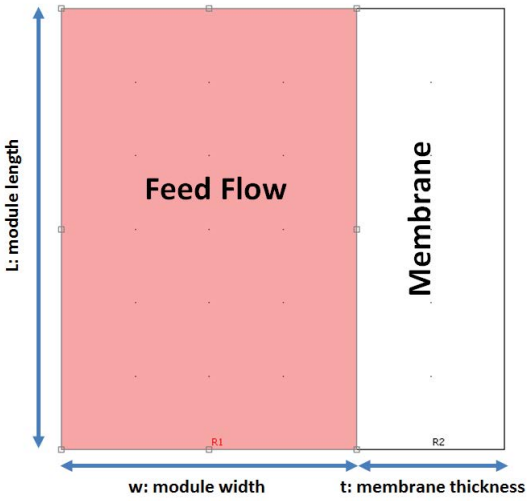

Fig. 1. Model geometry for computational simulation.

The membrane processes have been extensively used in literature for separation and purification of aqueous liquid and gas streams and theoretical and experimental analysis are available for modeling and numerical simulation of the process. Finite element method (FEM) was used to solve the problem. The mass transfer in the polymer is Maxwell–Stefan's diffusion.

A mechanistic model is developed here in order to track the different quantities of interest for the process such as concentration, velocity, and pressure. It has already reported in the literature that the concentration continuity equation along with thermodynamic approaches is a great tool for modeling of chemical processes. Therefore, conservation equation can be written as [38]:

$$\frac{\partial C_w}{\partial t} + \nabla \times \left(J_w + C_w V \right) = R_w \tag{1}$$

The reaction term is omitted as there is no chemical reaction involved in this process.

2.1. Numerical calculations

The derived equations of the model [Eq. (1)] are numerically solved by appropriate solver and conditions in order to simulate the process. As a starting point, the whole geometry of model needs to be discretized which is shown in Fig. 2. In this study, FEM was coupled with adaptive meshing and error control using numerical solver of UMFPACK version 4.2.

3. Results and discussion

The concentration of the solute in the process is shown in Fig. 3 as a colorful two-dimensional distribution which has been obtained by numerical solution of Eq. (1) using computational fluid dynamics approach. Fig. 4 also shows the contour of diffusive flux. The approach seems to be efficient in the modeling of the process and the concentration distribution of different species can be easily calculated in the process. Therefore, the methodology developed in this work is capable of prediction and optimizing the chemical separation processes.

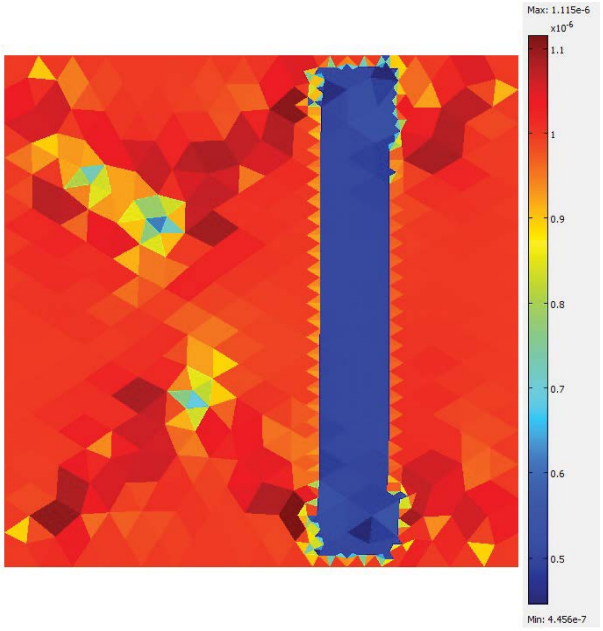

Fig. 2. Mesh element size used in the computations.

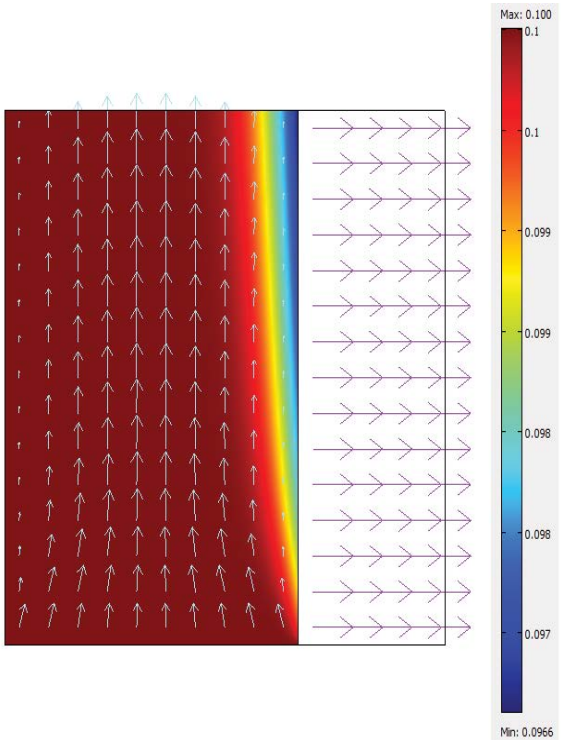

Fig. 3. Concentration distribution and arrows of total mass transfer flux of solute.

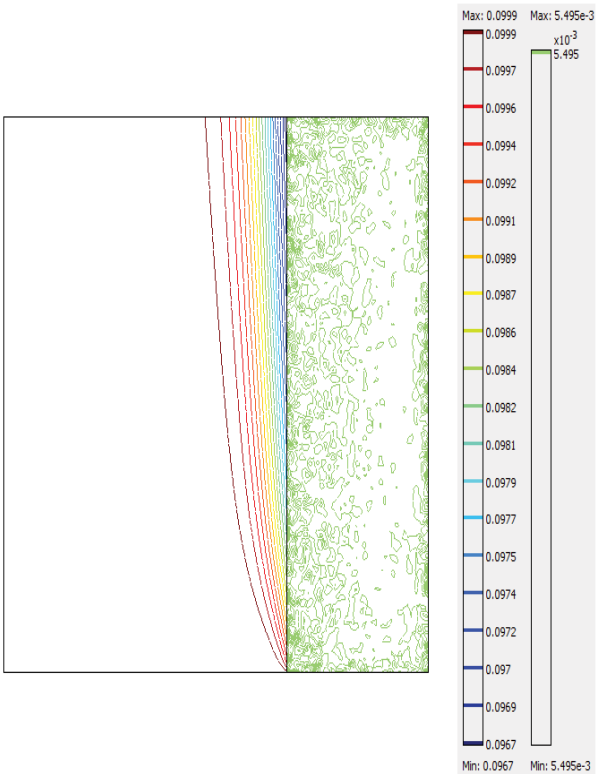

Fig. 4. Contours of diffusive flux inside the membrane and total flux of solute in the feed side.

4. Conclusions

A numerical methodology has been developed in this study in order to simulate the chemical separation processes used for purification and isolation of chemical compounds. The considered process is a membrane-based separation in which the equations of conservations were derived and numerically solved for various species in the process. The governing equations were then solved using the computational fluid dynamic approach in order to calculate the concentration of species in the process. The results indicated that the methodology is robust and efficient and can be used for computational modeling of processes.

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