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A general predictive model for sweeping gas membrane distillation

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ABSTRACT

Among the configurations of membrane distillation processes, sweeping gas membrane distillation (SGMD) remains one of the less studied. In spite of an increasing number of publications, generally the modeling of SGMD has been carried out by fitting heat and mass transfer coefficients and with the use of empirical correlations. In this work, a general predictive model based on computational fluid dynamics (CFD) is presented. This model allows simulating hollow fiber and flat sheet configurations under wide range of process conditions; with a minimum number of input data and without requiring empirical parameters or laboratory experiments. For this purpose, the momentum, mass and heat balances of the process are described by partial differential equations, algebraic and ordinary differential equations. The model has been validated with experimental results available in the literature. Indeed, the influence of operating conditions and membrane geometric characteristics on the process performance was investigated. The conducted studies prove that the proposed model would be potentially applied for the optimization of process conditions, design of membrane modules as well as for the further cost estimation of the process.

1. Introduction

Sweeping gas membrane distillation (SGMD) is a thermally driven process in which separation takes place on a membrane-liquid interface due to a phase change of volatile compounds. A basic SGMD unit consists of two channels separated by a flat sheet or hollow fiber hydrophobic membrane (Fig. 1). A liquid (generally an aqueous solution) is introduced in the upstream feed channel; whereas the downstream permeate channel is fed with a sweeping gas (SG). Indeed, the feed liquid does not wet the membrane and its volatile components evaporate at the interface created at the entrance of membrane pores [1]. The difference of the partial vapor pressure between the upstream and downstream flows allows the diffusion of volatile compounds through the membrane pores towards the permeate side and leave the SGMD unit with SG. The volatile compounds can eventually be condensed outside the membrane unit.

SGMD, which requires large amounts of SG, external condenser and related costs, is the least studied membrane distillation (MD) configuration [2]. According to Essalhi and Khayet [3], at the end of 2013, only 4.6% of publications related to MD were dedicated to SGMD, and, to the best of our knowledge, this trend continues until today. Despite this low number of publications, SGMD has already proved its possible application in desalination, including the works of Basini et al. [4], Khayet et al. [5–8] and Charfi et al. [9]. However, the application of this process has been mainly explored for a lot a different purposes: removal of volatile organic compounds from dilute aqueous solutions [10–13] (in several studies SGMD was also named as membrane air stripping), ammonia removal from water and wastewater [14], recovery of volatile fruit juice aroma [15], removal of formic acid [16], separation of aqueous solutions from aromatic compounds [17], triethylene glycol – waste water separation [18] and concentration of thermally sensitive solutions [19–22].

Several mathematical models have been proposed to simulate the SGMD process. Khayet et al. [23, 24] had proposed a two-dimensional SGMD model which uses empirical heat transfer coefficients, experimental data for solving procedure and integral equations to describe simultaneous transmembrane heat and mass transfer. In a further work [25], the calculation of the temperature profiles of the feed and permeate sides was simplified to estimate the bulk and boundary temperatures of the fluids. By using the proposed models, Khayet et al. have investigated transmembrane water vapor flux, membrane surface temperature and temperature polarization (TP) and conducted a parametric study, including the feed and permeate temperatures, feed and permeate velocities and salinity of the feed liquid. It is worth noting that such modeling approach to describe simultaneous heat and mass transfer by the integral equations with the application of the empirical correlations and use of experimental data is the most popular in the literature [26–33]. However, these models have a limited application in

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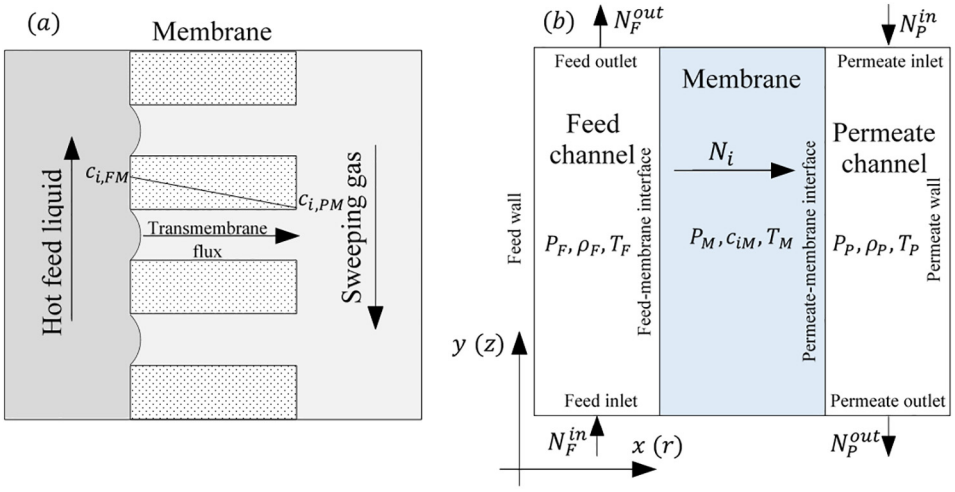

Fig. 1. (a) Schematic representation of SGMD and (b) schematic representation of the parameters considered in the model. P_F, P_P, P_M and T_F, T_P, T_M are the pressures and temperatures in the feed, permeate and membrane domain respectively; ρ_F and ρ_P are the densities of the feed and permeate flows respectively; c_{iM} is the molar concentration of the component i in the membrane pores; N_i is the molar transmembrane flux of the component i; N_F^{in}, N_P^{in} and N_F^{out}, N_P^{out} are the total fluxes of the feed liquid and SG at the inlet and outlet of feed and permeate respectively.

the process design and module optimization due to the use of discrete lumped variables in the equations and the need of empirical or experimental data.

In contrast to the previous models, Charfi et al. [9] presented a computational fluid dynamics (CFD) model of SGMD. In such work, the momentum, mass and heat balances were presented in the form of the partial differential equations (PDEs) for the feed side, membrane media and permeate side. The CFD approach, which is allowed to use continuous distributed variables, reduces the dependence of the model on the empirical or experimental data and increases the level of physical description. Indeed, the velocity, concentration and temperature distributions in the SGMD module are calculated. The mentioned qualities of the CFD model make it suitable for the process design and the module optimization. Nevertheless, the model presented by Charfi et al. has some significant drawbacks: the use of the model is limited to the specific case where the feed and permeate fluids are binary mixtures; the effect of the concentration of SG on the effective diffusion coefficient is not included; the model takes into account transport of only a single component through the membrane; SG is presented as an incompressible flow; the momentum balance is determined only for the laminar flow; different compartments (feed channel, permeate channel and membrane) are combined in one domain. In addition, internal boundary conditions (BCs) responsible for the momentum, heat and mass transfer from the feed side to the membrane media and from the membrane media to the permeate side are not defined clearly. This last drawback is especially important because these BCs define the driving force of the process, evaporation rate of the volatile components into the membrane pores, concentration of the sweeping gas at the feed-membrane and permeate-membrane interfaces, heat transfer between phases and, therefore, the flow rate of the target components through the membrane and then, the performance of the process.

In this study, we propose a new general predictive model for SGMD. This model is independent on experimental data and allows calculating detailed velocity, concentration and temperature profiles extending the knowledge of the process. The model consists of the momentum, mass and heat balances which take the form of partial differential equations (PDE), algebraic equations (AE) and ordinary differential equations (ODE). The BCs characterizing inlets and outlets of the process unit, walls and feed-membrane and permeate-membrane interfaces, are defined for the individual domains of the SGMD module (feed side, permeate side and membrane). The model is suitable for both flat sheet and hollow fiber configurations and can be used for different SGMD applications. The multicomponent fluids with laminar, transient and turbulent flows are considered in feed and permeate compartments. Indeed, the dusty gas model (DGM) is used for the description of mass transfer trough the porous membrane [34, 35]. The solving procedure was done in COMSOL Multiphysics™ software (5.1) which uses the principle of the finite elements method. The model has been validated by comparison of literature data and simulations. The simulated results are in good agreement with the literature data. Moreover, the study of membrane length and thickness, for which there is no experimental data, allowed predicting the influence of these characteristics on the SGMD performance.

2. Model description

The proposed model can be applied for the both hollow fiber and flat sheet configurations. Both the dynamic and steady state regimes of work of SGMD are considered. The model defines three domains of the SGMD module: the feed channel, membrane and permeate channel (Fig. 1).

In the case of a module containing multiple hollow fibers, the momentum, mass and heat transfer at the lumen side of the hollow fiber has been considered similar for any single fiber in the module. However, in the shell side of the hollow fiber, these processes are complex and dependent on many parameters, such as the packing density, number of the hollow fibers in the module and distance between them. Thus, for that type of the SGMD modules, the proper simulation accounting all the mentioned parameters can be done only in 3D. This procedure is an extremely resource- and time-consuming task. To reduce the computational burden and intensify the calculation process of the mathematical model, the simulation of the whole SGMD module with numerous hollow fibers is transformed into the simulation of the part of the module with only one hollow fiber surrounded by a defined volume of shell side module (Fig. 2). This approach has already been successfully applied for the modeling of hollow fibers modules for liquid-liquid extraction processes [36–38]. The concept of the flow in pipe is considered in the lumen side of the membrane. To model the momentum, mass and heat transfer in the shell side of the membrane, we assume that the considered hollow fiber is equidistant from the surrounding hollow fibers as it is shown on Fig. 2b. In real situations (Fig. 2a) the distances between hollow fibers may vary. Then, we divide the cross-sectional area of the permeate channel (dash lines on Fig. 2b) in such a way that it formed annuli around the hollow fibers. For the modeled part of the DCMD module (one hollow fiber with the annular permeate channel), the feed and permeate flow rates are calculated in proportion to values used for the multiple hollow fiber module. Therefore, the flow rates of the feed and permeate fluids are calculated by the following equation:

$$\dot{m}_z = \frac{\dot{m}_{tz}}{n_M} \tag{1}$$