Desalination 445 (2018) 181–196

Contents lists available at ScienceDirect

Desalination

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

A general predictive model for direct contact membrane distillation

V. Perfilov[a,*], A. Ali[b], V. Fila[a]

[a] Department of Inorganic Technology, University of Chemistry and Technology, Prague 16628, Czech Republic
[b] National Research Council - Institute on Membrane Technology (ITM–CNR), Via Pietro BUCCI, c/o The University of Calabria, cubo 17C, 87036 Rende CS, Italy

ARTICLE INFO

Keywords:
Direct contact membrane distillation
General predictive model
Mathematical modeling
Computational fluid dynamics
Numerical simulation
Heat and mass transfer

ABSTRACT

Direct contact membrane distillation (DCMD) is a nonisothermal technology applied for the separation of non-volatile components from aqueous solutions. Nowadays, a huge number of publications are dedicated to modeling of DCMD, however all of the presented models have at least one of the following disadvantages: over-simplification, the use of empirical heat and mass transfer coefficients and poor prediction for cases which are out of the experimental data range. To overcome these drawbacks, a multipurpose general predictive model of DCMD has been developed. The proposed model is suitable for hollow fiber and flat sheet configurations with or without spacers. For each compartment of the DCMD process, our model describes the momentum, mass and heat balances by systems of ordinary differential, partial differential and algebraic equations. The performance of the model has been analyzed in terms of the operating parameters (concentration of a feed solution, feed flow rate and feed temperature) and membrane thickness and length. The simulated results were in very good agreement with experimental and literature data. The broad parametric study demonstrates the great potential of application of the proposed model not only in the process optimization but in design of DCMD modules.

1. Introduction

Membrane distillation (MD) is a relatively less-explored membrane process based on the application of a microporous hydrophobic membrane that allows the passage of volatile components only. This process has several advantages including the ability to concentrate the solutions to their saturation level, production of high-quality water from saline solutions and the ability to exploit low-grade heat for the operation. First mentioned in the 1960s [1–3], the process was standardized 20 years later [4,5]. Recently, there has been a massive increase in the number of articles focused on the improvement and application of MD. Nowadays, MD is considered to be a potentially interesting tool for desalination [6–13], wastewater treatment [14–20], concentration of acids [21,22], treatment of agro-food [23–26] and biological solutions [27–29]. For these applications, MD can be used as a standalone process or in combination with pressure driven membrane operations such as reverse osmosis [6].

In direct contact membrane distillation (DCMD), the most studied MD configuration, both hot feed and cold permeate solutions are in direct contact with a membrane (Fig. 1(a)). The driving force of the process is the transmembrane temperature difference, which creates a vapor pressure gradient. Thus, the molecules of the volatile compound evaporate at the feed-membrane interface, pass through the membrane and condensate at the permeate-membrane interface.

The initial studies dedicated to the modeling of DCMD were published in the 1980s [30–33]. These works used integral equations and empirical correlations to describe membrane heat transfer, membrane mass balance and possible types of trans-membrane flux (viscous flow, Knudsen flow and molecular diffusion). However, in those studies, the feed and permeate mass fluxes were not described and the feed and permeate domains were only characterized by heat fluxes and by bulk phase and boundary layer temperatures. Furthermore, the simulation results of these models can only be applied in specific cases of the conducted experiments and validity of defined empirical heat and mass transfer coefficients. Despite this, such models remained popular for more than a decade [34–43]. In fact, because of their simplicity, they are even still used today. In contrast to the aforementioned works, Laganà et al. [24] proposed a model that paid attention to the feed and permeate domains. This model supported existing models by supplying heat-balance, mass-balance and fluid dynamics for those domains, thereby considerably enhancing the precision of the calculations.

Another approach of the use of the existing integral equations for the heat and mass balances in DCMD was proposed by Ali et al. [48,49] and Gustafson et al. [50]. In their studies, the DCMD module is discretized its length into several segments. In each segment, the overall heat and mass balances for the feed, permeate and membrane are

* Corresponding author at: Technická 5, 166 28 Prague, Czech Republic.
E-mail address: perfilov@vscht.cz (V. Perfilov).

https://doi.org/10.1016/j.desal.2018.08.002
Received 5 March 2018; Received in revised form 29 July 2018; Accepted 2 August 2018

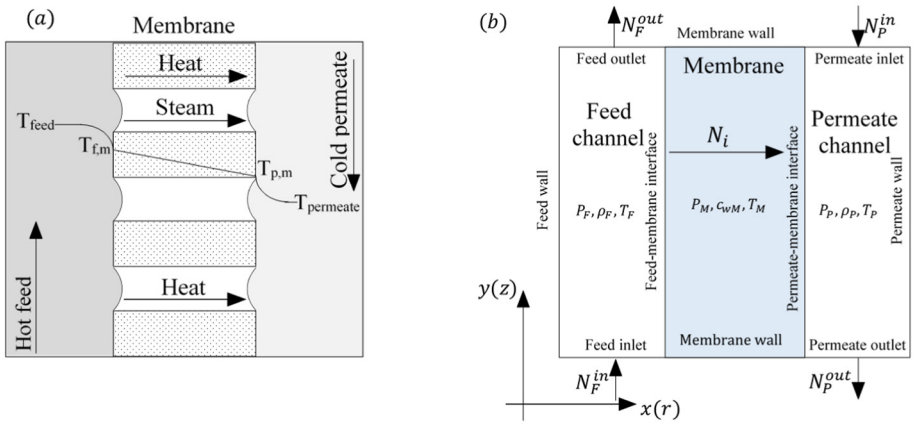

Fig. 1. (a) A schematic representation of the DCMD process and (b) a schematic representation of the DCMD modeling design.

determined. The balances of the current segment are connected to the previous and subsequent segments by heat and mass fluxes. This approach allows more accurate modeling of DCMD in comparison to the models where the whole DCMD module is presented by the one segment. However, the drawbacks typical for the existing models which use integral equations are still present and, to the best of our knowledge, the trend of the using the integral equations in the DCMD modeling still continues.

In the last decade, due to the rapid developments in information technology and huge scientific attention on simulation software, new models that use computational fluid dynamics (CFD) analysis were presented [44–47]. These studies used partial differential equations (PDE) to describe the mass, heat and momentum balances for the feed and permeate channels. Within these models, the finite element method (FEM) is used to create the velocity and mass flux profiles of these domains. However, the momentum, mass and heat balances of the membrane domain were still described by the same integral equations and empirical correlations, used in the previous studies, or by oversimplified PDEs. Another significant disadvantage of these models is that the boundary conditions between the membrane and liquids were not fully determined or described with the help of empirical heat and mass transfer coefficients. The use of experimental data in process modeling and analysis makes the existing models strongly experiment-dependent. Thus, these models remain unusable for the detailed simulation and prediction of behavior of DCMD units under width range of process parameters and/or the DCMD units having different geometry.

To eliminate the use of empirical heat and mass transfer coefficients, increase prediction of DCMD simulations and deepen our understanding of the process design of a DCMD unit, we propose a new general predictive model for DCMD. The model is applicable for hollow fiber and flat sheet membranes with empty as well as spacer filled channels. The mathematical model, based on mass, heat and momentum balances and mass transfer equations, results in systems of ordinary differential, partial differential and algebraic equations. The equations are solved using COMSOL Multiphysics™ software with use of a computational fluid dynamics (CFD) approach what improves the accuracy of the simulation. The effects of key parameters and membrane properties on the performance of a DCMD unit are also predicted and compared with the corresponding experimental data.

2. Theoretical description

The developed model allows simulation of DCMD with different geometries: i) the flat sheet configuration by using of Cartesian coordinates (Fig. 1(b)) and ii) the hollow fiber configuration by using of axisymmetric coordinates (Fig. 2(a)). Three different domains of the DCMD module are defined: the feed channel, permeate channel and membrane (Fig. 1).

For modules which contain multiple hollow fibers, the modeling of the whole DCMD unit can become a highly resource- and time-consuming process. To overcome this drawback, the calculation is transformed to the simulation of the DCMD process with one hollow fiber. In this case, feed flow and permeate flows are calculated in proportion to values used for the multiple fiber module. Therefore, the flows of the feed and permeate fluids are calculated by the following equation:

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

where $\dot{m}$ is the proportional total flow rate used in the module simulation, $\dot{m}_t$ is the total flow rate used in the real module, n_{HF} is the number of the hollow fibers in real module, z is the identifier of the side.

For the hollow fiber module, the proportional shell diameter of simulated domain is calculated by the following equation:

$$D_{Shell} = \sqrt{\left(\frac{A_{Shell}}{n_{HF}} + A_{OF}\right)\frac{4}{\pi}} \tag{2}$$

where A_{Shell} is the cross-section area of the shell side channel of the DCMD module, n_{HF} is the number of the hollow fibers, A_{OF} is the cross-section area taken by the one hollow fiber.

A similar approach can be used for flat sheet modules containing multiple frames (plate and frame modules). In this case, the model considers a half of the one feed channel, a half of the one permeate channel and a membrane between these halves (Fig. 2(b)). We also assume that the number of the feed and permeate half-channels is equal to number of membrane in the plate and frame module. Therefore, the feed flow rate and the permeate flow rate in one half-channel are calculated from the following equations:

$$\dot{m}_F = \frac{\dot{m}_{TF}}{n_{FS}} \tag{3}$$

$$\dot{m}_P = \frac{\dot{m}_{TP}}{n_{FS}} \tag{4}$$

where $\dot{m}_{TF}$ is the total feed flow rate, $\dot{m}_F$ is the feed flow rate in one channel, n_{FS} is the number of membranes in the plate and frame module, $\dot{m}_{TP}$ is the total flow rate of the permeate liquid, $\dot{m}_P$ is the flow rate of the permeate liquid in one channel.

The DCMD flow pattern in the model can be set to both co-current and counter current. For each part of the DCMD module, the momentum, mass and heat balances are described by the systems of the equations derived for the dynamic state. However, these equations could be easily simplified to the steady state conditions.