Journal of Membrane Science 515 (2016) 63–78

Contents lists available at ScienceDirect

Journal of Membrane Science

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

Calibration and analysis of a direct contact membrane distillation model using Monte Carlo filtering

I. Hitsov [a,b,*,1], L. Eykens [b,c,1], K. De Sitter [b], C. Dotremont [b], L. Pinoy [d], B. Van der Bruggen [c], I. Nopens [a]

[a] BIOMATH, Department of Mathematical Modelling, Statistics and Bioinformatics, Faculty of Bioscience Engineering, Ghent University, Coupure Links 653, 9000 Ghent, Belgium
[b] VITO - Flemish Institute for Technological Research, Boeretang 200, 2400 Mol, Belgium
[c] Department of Chemical Engineering, Process Engineering for Sustainable Systems Section, KU Leuven, W. de Croylaan 46, 3001 Leuven, Belgium
[d] Department of Chemical Engineering, Cluster Sustainable Chemical Process Technology, KU Leuven, Gebroeders Desmetstraat 1, Ghent B-9000, Belgium

ARTICLE INFO

Article history:
Received 19 February 2016
Received in revised form
28 April 2016
Accepted 17 May 2016
Available online 28 May 2016

Keywords:
Membrane distillation
Heat transfer
Mass transfer
Monte Carlo
Improved accuracy

ABSTRACT

Membrane distillation is an emerging technology to separate non-volatile components from an aqueous feed stream. Mathematical models have proven useful to pursue breakthrough in the economics of the technology and for further improvement through module design and operational optimization. However, before this can be done, all of the resistances in the system must be identified correctly and the model must be carefully calibrated to ensure its predictive power.

In this work the typical structure of a direct contact membrane distillation (DCMD) model is studied, where the mass transfer inside the membrane is simulated using the Dusty Gas Model and Nusselt type equations are used to simulate the heat transfer inside the channels. We demonstrate that an off-the-shelf Nusselt equation cannot directly be applied to simulate the heat transfer in the spacer filled channels. Instead, the equations should be calibrated to match the behaviour of the particular spacer.

A Monte Carlo filtering method was applied to calibrate and study the structure of the DCMD model for the membrane region. The method proved useful to identify which parameters need to be included in the calibration as it highlighted parameter correlations. Additionally, a submodel selection was performed for the heat and mass transfer inside the membrane.

A simple, yet physical method for the simulation of supported membranes was tested and validated on 3 supported membranes, resulting in an excellent fit.

1. Introduction

Membrane distillation is a thermally driven separation process in which the volatile components are transported through a porous hydrophobic membrane due to a vapor pressure gradient [1]. Meanwhile the non-volatile components exhibit almost absolute rejection [2,3].

In order to optimise the system, thorough knowledge is required. Process modelling is a powerful tool often used to build this system knowledge and can highly contribute to optimize these systems. Membrane distillation modelling can be found in many papers [4–6], but how the model was calibrated is rarely discussed. In our view, proper calibration, followed by a validation is key to good modelling practice and is often getting too little attention. If a model is not calibrated correctly and for example the mass transfer is overcompensating for the heat transfer, just to achieve a good fit of the experimental data, the predictive power of the model could be sufficient. However, such an overfitted model cannot be used to study what is the limiting resistance in the system and is very likely to fail if the model is scaled up beyond lab-scale dimensions. Therefore it is crucial that all the heat (HT) and mass (MT) resistances in the system (Fig. 1) are calibrated properly.

1.1. Transport phenomena in the channels

Nusselt equations are commonly used in membrane distillation modelling to simulate the heat transfer inside the fluid-filled channels [7,8]. The Nusselt equations are semi-empirical

* Corresponding author at: VITO - Flemish Institute for Technological Research, Boeretang 200, 2400 Mol, Belgium.
E-mail addresses: Ivaylo.Hitsov@ugent.be (I. Hitsov), Lies.Eykens@vito.be (L. Eykens), Kristien.DeSitter@vito.be (K.D. Sitter), Chris.Dotremont@vito.be (C. Dotremont), Luc.Pinoy@kuleuven.be (L. Pinoy), Bart.VanderBruggen@cit.kuleuven.be (B.V.d. Bruggen), Ingmar.Nopens@ugent.be (I. Nopens).
[1] Both authors contributed equally to this work.

http://dx.doi.org/10.1016/j.memsci.2016.05.041
0376-7388/

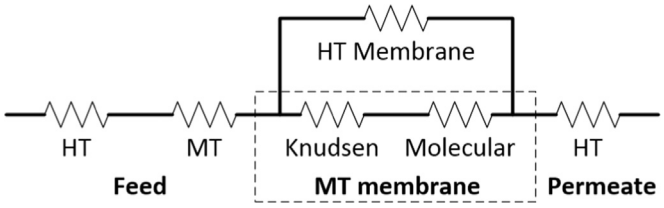

Fig. 1. Heat (HT) and mass transfer (MT) resistances in the DCMD system.

mathematical equations that were initially developed for heat transfer simulation in heat exchangers. The drawback of the Nusselt equations is that they are dependent on the flow regime and the geometry of the heat transfer surface. This results in hundreds of different relations specific for each case. However, in MD modelling these equations have rarely been validated [9,10] and instead a generic, off-the-shelf form is commonly used, but as shown by Tamburini et al. [11,12] each specific spacer has a Nusselt equation that describes its behaviour best. Hence, a generic form does not work for all spacers. In this work we utilize the methodology for spacer characterization of Phattaranawik et al. [10] where the membrane is replaced by an aluminium foil and the system is operated as heat exchanger at different flow velocities. Phattaranawik et al. then chose the best performing Nusselt equations from the literature. In this work, we take this approach a step further and calibrate a Nusselt equation to match the specific heat transfer behaviour of a spacer, instead of just choosing an expression "off-the-shelf".

Similar to the temperature polarization that occurs inside the MD channels, concentration polarization will also occur in the feed channels of a module - i.e. the salt concentration on the membrane surface will be increased due to the flux. It is commonly regarded that the concentration polarization in membrane distillation is not as important as thermal polarization [13], yet the research of Martínez et al. [14] demonstrates that at high salinities the concentration polarization resistance becomes important and should not be neglected. This resistance is calculated using the Sherwood number (Sh), a dimensionless number which is the mass transfer equivalent of the Nusselt number. However, these equations face the same applicability problem as the Nusselt equations since they are also specific to the geometry and flow regime [15]. In this work the similarity between heat and mass transfer is recognized, also known as the Chilton-Colburn analogy [16], which allows for a Sherwood type equation to be derived in complete analogy with the Nusselt equation based on the calibration of the heat transfer experiments.

1.2. Transport phenomena inside the membrane

The calculation of the heat transfer inside the membrane depends on the thermal conductivity of the membrane matrix. The conductivity of the membrane matrix is important for the calculation of the Energy Efficiency (EE), but it also affects the flux due to the additional temperature polarization that the membrane conductivity is introducing. This parameter however is difficult to measure, due to the possibility of membrane compression during the measurement [17]. Moreover, the thermal conductivity of the membrane matrix κ_m can be calculated using different models [18], but these are all developed for a certain pore orientation and membrane morphology [4]. Due to the large uncertainty of both measurement and calculation, possibly the thermal conductivity of the membrane κ_m can potentially be used as a calibration parameter in the model, but this has not been attempted before in the literature.

The Dusty Gas model (DGM) has been commonly applied in order to simulate the flux of vapors inside the porous membrane [19–21,14,7,22]. This model can predict the permeability of the membrane, based on the structural parameters such as porosity (ϵ), tortuosity (τ) and mean pore radius (R_p).

However, the DGM does not differentiate where exactly in the Knudsen-molecular transitional region a certain pore size is. To tackle this problem a model was recently introduced by Field et al. [23], which amends the DGM for the transition zone in order to correct the transitional DGM behaviour based on the Knudsen number, but this model has not been previously compared to the traditional DGM. The mass transfer inside the membrane can also be modelled using the Knudsen diffusion, molecular diffusion as well as a simple permeability constant. Therefore in this study a proper model selection was performed to evaluate the goodness-of-fit of these models.

Another common practice is to use the tortuosity of the membrane as a single calibration parameter for the membrane permeability [4]. However, a proper model structure analysis has not been performed thus far in the literature, to show if the other parameters in the DGM also require adjustments in order to obtain a good-fitting model.

To address the abovementioned problems, a rigorous Monte Carlo filtering method was applied for the first time to the model structure for the membrane region. Monte Carlo simulations are commonly used in many fields of science and engineering e.g. hydrology and wastewater treatment, to study model uncertainty and analyse the model structure [24–27]. In this work a goal function was defined to evaluate the quality of fit of the model to both the flux and the energy efficiency, which has not been done before in the literature but is common practice when a model is fitted to multiple experimental datasets, commonly known as multicriteria analysis [28]. The method was then applied according to good modelling practice principles and in order to:

- Study if the tortuosity is sufficient as a single calibration parameter for the membrane permeability or the other morphological parameters of the membrane also need to be included in the calibration.
- Investigate possible interactions between calibration parameters, i.e. parameters that counteract each other and multiple (infinite) combinations of their values result in the same quality of fit.
- Investigate whether the thermal conductivity of the membrane should be included in the calibration of the model.
- Perform a model selection for the sub-models that calculate the heat and mass transfer inside the membrane.
- Investigate the feasibility of a newly proposed method for simulation of supported membranes.

Furthermore, the method can later be used as a tool for automatic calibration and validation of the model. Following the presented method one can arrive at a model, where all of the resistances are identified correctly.

The applicability of the calibration method was demonstrated on 4 single layer and 3 supported membranes. Based on the Knudsen number all 7 membranes fall in the transitional regime between Knudsen and molecular diffusion.

2. Materials and methods

2.1. Membranes and module

The experimental data used for calibration were obtained in a flat sheet lab-scale MD setup (6×18 cm). Two channels with thickness of 2 mm each are formed by compressing two 60° spacers (Fig. 2) around a single membrane. The feed and the