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Open-source predictive simulators for scale-up of direct contact membrane distillation modules for seawater desalination

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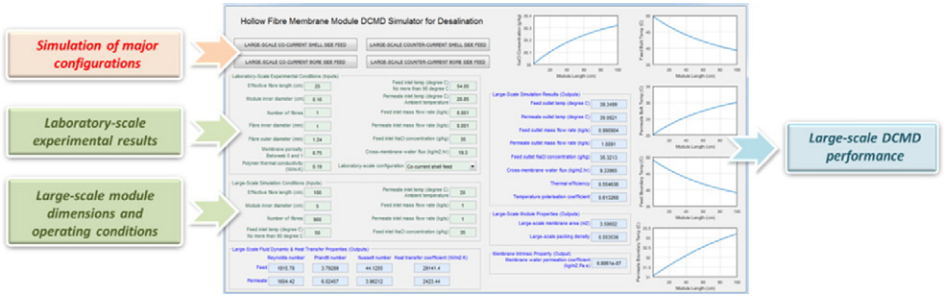
HIGHLIGHTS

- Two open-source simulators were developed for DCMD module scale-up.
- A coupled "tanks-in-series" and "black box" approach was developed.
- The developed simulators offer good accuracy.
- Profiles of major DCMD parameters versus membrane length were obtained.
- Key DCMD module scale-up criteria were identified and evaluated.

GRAPHICAL ABSTRACT



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ABSTRACT

Proper industrial-scale module design for seawater desalination by means of direct contact membrane distillation (DCMD) can be aided by module simulation. Accordingly, two open-source simulators (of flat sheet membranes and hollow fibre membranes) were developed on the Matlab GUI platform to supplement DCMD module scale-up. A coupled "tanks-in-series" and "black box" mathematical approach was developed not only to yield accurate simulation, but also to produce profiles of all the key parameters versus membrane length. Using laboratory-scale experimental results in one configuration as simulation inputs, the developed simulators were able to predict large-scale DCMD module performance in both co-current and counter-current configurations. These predictions exhibited good accuracy in both laboratory-scale and large-scale. Design considerations informing appropriate module scale-up for the DCMD process were demonstrated using the simulators. Key design criteria for industrial-scale module design were identified and evaluated. The results presented in this study offer general and practical guidance for proper module scale-up to deliver optimal pure water productivity for industrial-scale seawater desalination using the DCMD process. More importantly, the developed simulators are open-source, available for all researchers to develop specific DCMD module scale-up strategies for their own membranes.

1. Introduction

The direct contact membrane distillation (DCMD) process is a promising alternative means of seawater desalination, as (i) it can utilise waste-grade heat; (ii) its capacity is not limited by seawater salinity, unlike the conventional pressure-driven reverse osmosis (RO) process; and (iii) it allows the production of ultra-pure water. In a typical DCMD setup for

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seawater desalination, water molecules first evaporate at the gas-liquid interface of the hot feed stream, which then diffuse through the non-wetted membrane pores, and eventually condense in the cold permeate water stream [1–3]. The driving force for this process is the difference in vapour pressure across the membrane, which is governed by the solution temperatures in the boundary layers adjacent to the membrane surface. These boundary layer temperatures (T_{fm} and T_{pm}) usually differ greatly from the bulk temperatures (T_{fb} and T_{pb}) due to temperature polarisation, thus resulting in a much lower actual driving force (T_{fm}–T_{pm}) than the theoretical driving force (T_{fb}–T_{pb}) [4]. Because of the boundary layer temperature difference across the membrane, heat transfer takes place simultaneously with mass transfer. However, only a portion of the heat flux, the latent heat of vaporisation (q_v), contributes to mass transfer, whereas the accompanying conductive heat flux (q_c) causes an undesired additional heat loss, and therefore should be minimised. Thermal efficiency (the ratio between the latent heat and the total heat flux) is commonly used to indicate the proportion of heat transfer being utilised for pure water production.

The design of a DCMD module yielding high water productivity and optimal thermal efficiency requires a good knowledge of the heat and mass transfer in the DCMD process. However, the achievement of such a design is hindered by the lack of an effective non-intrusive experimental method for direct measurement of the boundary layer temperatures. This challenge can be tackled by using computer-aided simulation, which can predict the boundary layer temperatures as well as the heat and mass transfer behaviour inside a membrane module, thus providing critical information to supplement DCMD module design [5]. A number of modelling efforts have been reported previously, with Schofield et al. as one of the pioneering groups [6]. Since their work, extensive simulation studies have been carried out, mainly to provide fundamental understanding on heat and mass transfer mechanisms in the DCMD process, with topics including: (i) development of macroscopic models to describe mass transfer across the membrane for the prediction of membrane water permeation coefficient, with models developed including the Schofield model [7] and the dusty-gas model (which combines Knudsen diffusion, molecular diffusion, surface diffusion, and viscous flow) [8,9]; (ii) evaluation of existing semi-empirical correlations to appropriately describe the Nusselt numbers and the heat transfer coefficients [9–13]; (iii) proposal of new methods for the assessment of heat and mass transfer coefficients [14]; (iv) evaluation of heat and mass transfer, particularly heat transfer coefficients in hollow fibre geometry [15,16]; (v) study of the effects of various parameters upon heat and mass transfer, including membrane physical properties [17–19], the use of spacer-filled channels [10], process operating conditions (solution salinity, feed temperature, and flow rate) [12,20,21], and flat sheet membrane dimension [22]; (vi) multi-dimensional modelling, including two-dimensional modelling by means of computational fluid dynamics (CFD) simulation [16,23] or a coupling of a finite difference method (FDM) with the Runge-Kutta method [24], as well as three-dimensional Monte Carlo modelling [17]; and (vii) simulation studies on improving energy efficiency by means of coupling DCMD and heat exchanger or other novel process designs [25–27].

Despite the great breadth and depth of coverage by these previous studies regarding heat and mass transfer mechanisms in the DCMD process, we note that most of these efforts have focused solely on laboratory-scale DCMD. The heat and mass transfer behaviour observed in these simulation studies is thus unsuitable to be directly translated into or extrapolated to large-scale DCMD modules. Therefore, as a crucial step towards commercialisation of the DCMD process for seawater desalination, it is of great interest to develop a predictive simulator for large-scale DCMD module heat and mass transfer, which would provide critical guidance for appropriate module scale-up. However, to the best knowledge of the authors, only a handful of studies have been conducted so far to predict the performance of scaled-up DCMD modules [28,29]. Furthermore, source code from the models developed in these studies was not made available to public. This lack of access for other researchers has severely limited the impact of the previous works within membrane research.

Unlike most past simulation efforts, in which the models were specifically designed to guide laboratory-scale membrane material development for better DCMD performance, the current work instead aimed to develop two open-source user-friendly simulators (for flat sheet membranes in the plate-and-frame configuration and for hollow fibre membranes) to aid in DCMD module scale-up for seawater desalination. The developed simulators used laboratory-scale experimental results from one configuration as simulation inputs to predict the performance of scaled-up modules in several commonly used configurations, including co- and counter-current configurations, as well as shell- and bore-side feeds (for hollow fibre modules). A coupled "tanks-in-series" and "black box" mathematical approach was developed to establish profiles of all key DCMD parameters versus membrane length. The developed simulators were then used to predict the desalination performance of industrial-scale flat sheet and hollow fibre modules, and the effects of membrane physical properties, module dimensions, and operating conditions upon large-scale DCMD module performance were evaluated to demonstrate critical design considerations yielding DCMD module scale-up for optimal pure water productivity.

2. Simulator development

The "tanks-in-series" mathematical model has been applied for membrane separation simulations, mainly for gas separation through either flat sheet or hollow fibre membranes [30,31]. In this study, the same approach was adopted; the membrane module was divided into a series of tanks of equal axial length of 1 cm (Fig. 1). With such an approach, profiles of heat and mass transfer rates, feed concentration, flow rates, cross-membrane water flux, and bulk and boundary layer temperatures can be established as a function of effective membrane length.

The following assumptions were made during the development of the simulators reported herein:

- No membrane wetting takes place, and 100% salt rejection is assumed,
- The developed simulators treat the DCMD process as a steady-state process,
- Fluid is fully developed, with entrance and exit effects neglected,
- The membrane module is perfectly insulated, so there is no heat loss to the surrounding environment,
- No spacer is used in membrane modules for the current flat sheet membrane simulator. (The effect of spacers upon fluid dynamics and heat and mass transfer will be evaluated in our future simulation work),
- A linear temperature gradient is assumed inside membrane matrix, as proven valid in previous modelling work [10],
- The concentration polarisation effect is assumed to be negligible, as proven valid in previous laboratory-scale experimental work [32]. (More advanced simulators considering the concentration polarisation effect will be developed in our future work).

We note that the DCMD performance can be affected by the pressure drop in large-scale modules, as it may lead to local pressures greater than the liquid entry pressure (LEP), thereby resulting in membrane wetting and reduced salt rejection. However, membrane wetting behaviour is difficult to simulate, as it is largely affected by the microstructural properties of the membrane itself. The current work assumes no membrane wetting, under which assumption, pressure drop will not affect the water flux and salt rejection aspects of DCMD performance. Nevertheless, we intend to include the effect of pressure drop in our future simulation work for its prediction to uncover possible indications of local membrane wetting, especially in the entrance region of large-scale modules.