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Improved analytic modeling and experimental validation for brackish-water reverse-osmosis desalination

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HIGHLIGHTS

- New analytical modeling with predictive accuracy confirmed by extensive experiments
- Predicts how permeate flow and salinity depend on pressure and feedwater properties
- No adjustable parameters, capturing the key physics of reverse osmosis operation
- Ability to predict, rather than assume a knowledge of, permeate concentration
- Required input information requires no more than standard manufacturer specifications

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ABSTRACT

We derive an expanded analytical model for the performance of brackish-water reverse-osmosis desalination systems, and conduct extensive measurements on a modest-sized laboratory system, over broad ranges of feedwater salinity and system driving pressure toward establishing good agreement between theory and experiment. The model has no adjustable parameters, captures the essential physics, casts the analysis in terms of the system's natural physically-transparent variables, and accounts for how permeate flow rate and permeate concentration vary with the principal control parameters: system driving pressure, feedwater flow rate and feedwater salinity. By explicitly and analytically incorporating salt diffusion across the membrane into the model, we show how accurate performance predictions can be made with no more input information than is commonly provided in manufacturer specifications. The predictive capabilities of the improved model are also elaborated — a cardinal point being the ability to *predict* permeate concentration rather than having to assume it as a known input parameter.

1. Introduction

Predicting the variation of flow rates and concentration levels through reverse osmosis (RO) desalination systems (Fig. 1) is typically performed with large-scale numerical simulations [1–3]. Here we focus on the alternative of capturing just enough of the essential physics — with relatively simple and physically transparent descriptions of the key system variables and their governing equations — to yield accurate predictions of the primary performance variables. Establishing model accuracy is based on performing the extensive experiments reported here on a small-scale laboratory brackish-water (BW) RO system, over a broad range of operating conditions, to wit, a factor of 3.0 in feedwater concentration C_f, and a factor of 1.8 in system entry pressure P. While numerous modeling studies [4–11] have elucidated the basic processes, their limitations include (a) invoking a large array of adjustable parameters that are unavailable *a priori*, (b) having to include complex fluid dynamic equations and boundary-layer theory, the numerical solution of which proves quite cumbersome, (c) relating only to pervaporation or organic-solute separation processes that are basically distinct from desalination, or (d) lacking wide-reaching experimental verification (specifically for desalination).

The analytical model reported in [12] for BWRO systems simultaneously (1) obviated the need for massive computer simulations; (2) provided a physically transparent picture that clearly identified the impact of each key design variable on system performance, cast in terms of two natural characteristic variables for length scale and flow rate; and (3) offered a predictive method that was shown to agree well with extensive experimental results for *low*-salinity BWRO. A central goal was predicting how the volumetric flow rate of the permeate (desalinated water) Q_p varies along the system, together with its dependence on P, feedwater C_f, and feedwater volumetric flow rate Q_f.

However, the model had two shortcomings that limit its value in accounting for RO system behavior: (a) requiring the permeate

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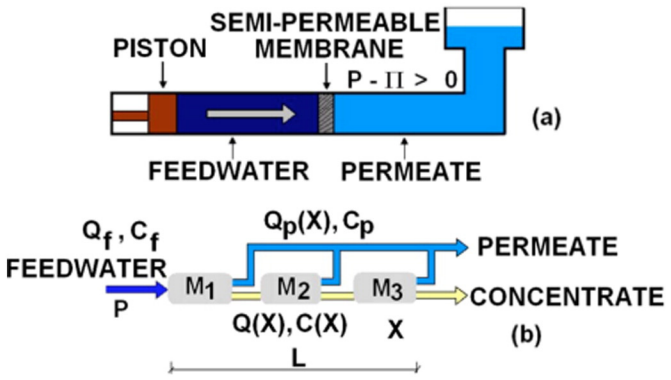

Fig. 1. RO schematic, illustrating (a) the pressure-driven mass transfer across an individual membrane, and (b) flow at an arbitrary length x along the membrane in a 3-stage (3-membrane M_1, M_2, M_3) system of known total membrane length L. Separate collection of permeate and concentrate is indicated. Other symbols are defined in the text.

concentration as known input, rather than predicting it from commonly available input parameters, and (b) prediction inaccuracies that grew non-negligible when feedwater salinity reached $C_f = 5$ g/kg (5000 ppm).

Here, we show how additionally introducing the explicit equation for solute diffusion across the membrane (1) permits an analytical solution that *predicts* the permeate concentration (rather than *requiring* it as a known input parameter), and (2) provides adequate predictions of system performance when compared against extensive experimental measurements up to the highest feedwater salinity level that could be treated in our BWRO system, $C_f = 6$ g/kg.

2. System basics and a review of the prior analytical model

We first review the analytical model of [12], in order to establish the basic physical picture, and to clarify precisely how the expanded analytical model of this paper provides a more powerful modeling capability. Referring to Fig. 1, we express the one-dimensional diffusion of salt across a membrane of length L at a given position x ($0 \le x \le L$) in terms of the conservation equations for salt concentration C and volumetric flow rate Q, along with the condition for the flow gradient, respectively:

$$C_f Q_f = C_p Q_p(x) + C(x)Q(x) \tag{1}$$

$$Q_f = Q_p(x) + Q(x) \tag{2}$$

$$\frac{dQ(x)}{dx} = -k_{per} w\left(P - f_{polar}\Pi(x) + \Pi_p\right) \tag{3}$$

where subscripts p and f respectively denote permeate and feedwater, no subscript is used for the concentrate, the *driving* and osmotic pressure are respectively denoted by P and Π, and w is the membrane's width.

f_{polar} is the dimensionless membrane polarization factor that accounts for the increase in ion concentration at the membrane surface as a consequence of ion diffusion from the bulk flow. f_{polar} can be assessed with analytical film theory [13–15], with an accuracy comparable to that of rigorous numerical diffusion-convection models [13]. Prior studies [12–15] have evidenced the approximate constancy of f_{polar} over a wide range of pressure for representative RO systems. Based on these studies, $f_{polar} = 1.15$ was estimated for the system analyzed here. As an independent consistency check, we used our experimental measurements and the model of [12] to compute f_{polar} over the broad span of operating conditions considered here, yielding f_{polar} values from 1.00 to 1.25. The fact that the approximation $f_{polar} = 1.15$ yields good performance predictions (*vide infra*) would therefore appear to augur well for the sufficiency of treating it as approximately constant at 1.15.

k_{per} is the membrane's permeability coefficient for water, typically of the order of 10^{-11} m/s/Pa [12,13], and provided by the manufacturer for prescribed inlet and operating conditions. At low P, where the transmembrane pressure is small (i.e., where $\Pi(L) - \Pi_p$ approaches P), k_{per} grows large in order to sustain the permeate flow. Typically, RO systems are not operated in this regime due to the combination of operational instabilities, the need for increased membrane area (more equipment) and hence greater cost, and the difficulty of reaching sufficiently low permeate concentration. These effects are exacerbated as C_f increases. (Indeed, the onset of perceptible differences between theory and experiment in the analyses reported below occurs at the highest C_f and lowest P values in the experiments.) Nonetheless, both experimental results and corresponding model predictions for this low-flux regime were covered toward examining model accuracy as the practical limits of BWRO system operation are approached.

As P increases, k_{per} decreases and eventually asymptotes, principally due to the effects of membrane compaction [1,16,17]. The narrow range of operating conditions in common RO desalination systems for the practical (asymptotic) higher-P realm permits approximating k_{per} as constant.

Additionally, Π can be well approximated by Van't Hoff's law:

$$\Pi = \nu_s R T C = K C \tag{4}$$

with R being the universal gas constant, and ν_s denoting the number of ions per salt molecule (e.g., $\nu_s = 2$ for NaCl). Since in the common configuration of spiral-wound modules the permeate is continuously mixed in a single vessel, the x-dependence of C_p and of osmotic pressure Π there can be neglected.

We can then combine and recast Eqs. (1)–(4) into a single linear differential equation

$$\frac{dQ(x)}{dx} = -\frac{Q_f}{\lambda}\left(1 - \frac{\Theta}{Q(x)}\right) \tag{5}$$

where the system's natural characteristic length scale λ and flow rate Θ are

$$\lambda = \frac{Q_f}{k_{per} w\left(P + \left(1 - f_{polar}\right)\Pi_p\right)} \qquad \Theta = \frac{Q_f f_{polar}\left(\Pi_f - \Pi_p\right)}{P + \left(1 - f_{polar}\right)\Pi_p}. \tag{6}$$

The implicit solution of Eq. (5) represents a nominally universal relation:

$$\frac{x}{\lambda} = \frac{Q_f - Q(x)}{Q_f} - \frac{\Theta}{Q_f}\ln\left(1 - \frac{Q_f - Q(x)}{Q_f - \Theta}\right) \tag{7}$$

(where the initial condition $Q(0) = Q_f$ has been used). RO plant operators often refer to a recovery factor RF defined as the fraction of feedwater collected as permeate, over the total membrane length:

$$\mathrm{RF} = Q_p(L)/Q_f = 1 - (Q(L)/Q_f)\,. \tag{8}$$

The limitation in predicting system performance with this model, however, is requiring an advance knowledge of C_p, with C_p being implicit in the system's natural characteristic length scale λ and flow rate Θ (Eqs. (5)–(6)). Furthermore, although model predictions for the variation of $Q_p(L)$ with both Q_f and P were excellent at $C_f = 2$ g/kg, the discrepancies between theory and experiment grew non-negligible at $C_f = 5$ g/kg [12]. It was principally the inability of the analytical model to *predict* (rather than assume) C_p, and, secondarily, the imprecision in predictions at intermediate salinity levels, that prompted this investigation.