



Modeling reverse osmosis element design using superposition and an analogy to convective heat transfer



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ABSTRACT

Accurate models for concentration polarization (CP), the buildup of solutes at the membrane–solution interface in reverse osmosis (RO) channels, are critical for predicting system performance. Despite its empirical success, many modeling approximations employed in the derivation of the often-used stagnant film model seem to limit the model's applicability to real systems. In addition, many existing models for CP use an average mass transfer coefficient with a local mass transfer driving force, which leads to incorrect predictions for the osmotic pressure at the membrane–channel interface. In this work, we reduce the Zydne y-transformed governing equations for solute mass transfer to an analogous convective heat transfer problem. We then apply the principle of superposition to fit solutions from the heat transfer problem to the RO channel boundary conditions, yielding a solution that correctly and consistently combines a local transport coefficient with a local mass transfer driving force. The resulting expression for RO element sizing and rating shows good agreement with experimental data and provides a theoretical basis for CP modeling that captures the characteristic growth of the mass transfer boundary layer not accounted for by many existing, more empirical models. The model has important consequences for the design of RO systems with high permeability membranes, as the decrease in membrane resistance in these systems leads to a relative increase in the importance of CP in system performance.

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1. Introduction

In reverse osmosis (RO), the rejection of solutes by the membrane causes a buildup of solutes at the membrane surface, which increases the local osmotic pressure and retards water flux through the membrane. This phenomenon is known as concentration polarization (CP). Accurate prediction of the osmotic pressure—or equivalently, the solute concentration—at the membrane surface in RO systems is thus a critical problem for predicting the permeate flux, which in turn is essential for membrane sizing and techno-economic optimization. Good models for CP are even more important in systems using ultrapermeable membranes (UPMs) [1–3], as the higher permeability leads to a relatively larger mass transfer resistance from CP. In addition, high solute concentrations at the membrane surface can lead to fouling or scaling, which reduce the effective membrane surface area and increase maintenance cost. With improved predictability of solute concentrations at the membrane, such issues can be better prevented.

Almost 50 years ago, Michaels [4] applied the stagnant film model to specify the solute concentration at the membrane surface as a function of the bulk concentration and the permeate flux. Despite its analytical simplicity, the classic stagnant film approach involves several limitations, including the use of a conductive-like mass transfer coefficient and a wall-normal velocity that is invariant through the mass transfer boundary layer. The details of the approximations used to develop of the stagnant film model will be presented in Section 2.

Many improved analyses of concentration polarization in membrane channels are based on simplified mass transfer equations allowing for analytical or semi-analytical solutions of the problem [5–9]. However, most of these models are still limited by modeling approximations such as a constant permeate flux through the boundary layer and an axially invariant permeate flux. Further, many models rely on empirical correlations for the mass transfer coefficient, and/or incorrectly link an average mass transfer coefficient with a local driving force. Numerical methods [10–13] have been applied to overcome the drawbacks associated with the simplified models, but are computationally intensive and can be difficult to generalize.

The contribution of this paper is threefold. First, following the approach of Zydne y [14], we transform the governing species

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conservation equations to derive a model for concentration polarization that mathematically resembles the stagnant film, but which relaxes several of the often-stated modeling approximations. Second, we show how, under certain conditions, mass transfer coefficients for the film can be obtained by analogy to convective heat transfer, a subject for which a vast theoretical and experimental literature is available. Finally, we use the principle of superposition to develop a new model for membrane performance (recovery ratio or permeate flux) as a function of operating conditions, system geometry, and mass transfer coefficients. The latter are obtained from constant wall flux solutions to the governing transport equations. Results from the model are benchmarked against measurements, existing models in the literature, and solutions from direct numerical simulation. The results show better predictive performance at high degrees of concentration polarization, as would be found in systems with UPMs.

2. Development of the stagnant film model

A stagnant film (Fig. 1) assumes that there are no axial variations in the mass transfer boundary layer (MTBL) thickness, the solute concentration, and the solvent flux, leading to a 1-D problem. Application of the stagnant film model to concentration polarization was first presented by Michaels [4] and is derived by balancing the convective solute flux ($\rho v_n w$) towards the membrane with the counter-diffusive flux of solute away from the membrane that results from membrane solute rejection. Axial variations in both the permeate velocity and the solute concentration gradient are neglected, resulting in the following equation for species conservation:

$$\rho v_n w - \rho D \frac{dw}{dn} = 0, \quad (1)$$

where n is the unit vector that points normal to the membrane surface into the solution and $-v_n$ is the permeate velocity or volumetric flux. The mixture density is denoted ρ , w is the solute mass fraction, and D is the diffusivity of the solute in the solvent. Although the typical RO feed may contain multiple solutes, here we lump them together, modeling solute diffusivity with a single value D .

Taking the permeate velocity as constant through the MTBL allows Eq. (1) to be integrated across the MTBL thickness δ , yielding the proportionality between the permeate flux and the logarithm of the bulk-to-wall concentration ratio that is the hallmark of the stagnant film model:

$$v_n = \frac{D}{\delta} \ln \left(\frac{w_w}{w_b} \right). \quad (2)$$

The term D/δ is the mass transfer conductance based on the logarithmic concentration driving force, and is constant in the stagnant film model.

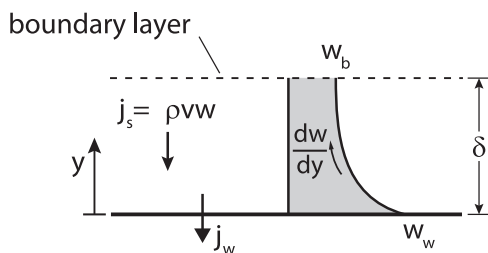


Fig. 1. As the solute is pulled convectively towards the wall, j_s , under the influence of the solvent suction through the wall, j_w , a counter-diffusive flux of the solute back towards the bulk develops. In a stagnant film, all properties vary only in the y -coordinate.

However, in long but narrow membrane channel flows, the concentration boundary layer can grow to cover a significant portion of the—or even the entire—channel height. Some key limitations of the stagnant film model mentioned in literature (see, e.g., [9,15] for a description) revolve mostly around the simplification to 1-D, and include:

- neglecting axial convection near the membrane surface,
- neglecting the influence of the permeate flux on the boundary layer thickness,
- neglecting axial variation in the permeate flux,
- assuming fully developed velocity and concentration profiles.

In spite of these limitations, however, models that use a logarithmic driving force to characterize the diffusion of solute across the MTBL have achieved considerable predictive success. In the following section, we follow the approach of Zydney [14], who showed that the mathematical form of the stagnant film model, albeit with a different mass transfer coefficient, can be derived using far fewer approximations than those listed above.

3. Zydney's transformation and the analogous heat transfer problem

3.1. Transformation using a pseudo-concentration

Zydney [14] uses a transformation of variables to show that the logarithmic concentration driving force that characterizes the stagnant film model is the correct driving force for the coupled convective and diffusive transport near the membrane surface. In this section, we adhere to Zydney's general idea [14] that validates the form of the stagnant film model by transforming the transport equation of a passive scalar (the solute). For simplicity, but without loss of generality, the governing equations are presented in two dimensions. For a spatially invariant density, the species conservation equation can be written in terms of solute mass fraction w , which yields

$$\frac{\partial w}{\partial t} + u_x \frac{\partial w}{\partial x} + u_y \frac{\partial w}{\partial y} = D \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right), \quad (3)$$

where $\vec{u} = (u_x, u_y)$ is the velocity field and D is the mass diffusivity of the solute in the solution. At the permeable boundary, i.e., the membrane surface, the no solute flux boundary condition is

$$-\rho D \frac{\partial w}{\partial n} - \rho w v_n = 0. \quad (4)$$

A non-zero term on the right hand side of Eq. (4) can be added to account for solute permeation through the membrane, but we will restrict ourselves to the case of full solute rejection for simplicity.

Along the impermeable boundary or a symmetry plane, there is no solute flux:

$$\frac{\partial w}{\partial n} = 0. \quad (5)$$

For the case that density changes by the solute/solvent mixture are small (i.e., $D\rho/Dt = 0$), the x and y momentum equations read, respectively

$$\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\mu}{\rho} \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right), \quad (6)$$

$$\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{\mu}{\rho} \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right), \quad (7)$$

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