Supplementary Information

Desalination by Forward Osmosis: Identifying Performance Limiting Parameters through Module-Scale Modeling

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Numerical Analysis of a Counter-Current FO Module

Fig. A1 depicts a FO membrane module of area A_m that has been discretized into N elements each of area A_m/N. N is selected in terms of A_m, the inlet feed flow rate, Q_{F0}, and a water flux, $J_{w,id}$:

$$N = \text{round}\left(\frac{512 A_m J_{w,id}}{Q_{F0}}\right) \tag{S1}$$

where $J_{w,id}$ is the water flux which would be obtained between the inlet feed and draw streams in the absence of concentration polarization and solute flux (i.e., $J_{w,id} = \nu A R_g T(c_{D0} - c_{F0})$). (The pre-factor of 512 in Eqn. (S1) is chosen such that there is no change to 4 significant figures in the numerical results of the model.)

The inlet flow rate and concentration of the feed stream, Q_{F0} and c_{F0} respectively, are known whilst the neighbouring outlet flow rate and concentration of the draw stream, Q_{D1} and c_{D1} respectively, are unknown. To solve the model we need to determine Q_{D1} and c_{D1} such that the calculated inlet flow rate and concentration of the draw stream, $Q_{D(N+1)}$ and $c_{D(N+1)}$ respectively, are within a 10^{-3} tolerance of known quantities Q_{D0} and c_{D0}.

Derived from the permeability-selectivity trade-off, Eq. (7) of the main manuscript relates the molar leakage rate of solute, ΔN_s, to the volumetric permeation rate of water, RQ_{F0}:

$$\frac{\Delta N_s}{RQ_{F0}} = \frac{B}{\upsilon A R_g T} \tag{7}$$

By combining a mass-balance on the draw stream with Eq. (7) we can express c_{D1} in terms of Q_{D1}:

$$c_{D1} = \frac{Q_{D0} c_{D0} - \frac{B}{\upsilon A R_g T}(Q_{D1} - Q_{D0})}{Q_{D1}} \tag{S2}$$

Mathematically we may represent the solution of the counter-current module in terms of a function $f(Q_{D1})$ of Q_{D1} (amongst other parameters):

$$f(Q_{D1}) = Q_{D(N+1)} - Q_{D0} = 0 \tag{S3}$$

where $Q_{D(N+1)}$ is a another function of Q_{D1}.

To calculate $Q_{D(N+1)}$ for a given Q_{D1} we numerically integrated Eqs. (15) and (16) of the main manuscript using the fourth-order Runge-Kutta method RK4 with a constant step size in area of A_m/N.

$$\frac{dQ_F}{dA_m} = \frac{dQ_D}{dA_m} = -J_w \tag{15}$$

$$\frac{d(Q_F c_F)}{dA_m} = \frac{d(Q_D c_D)}{dA_m} = J_s \tag{16}$$

At each step we solve flux Eqs. (13) and (14) of the main manuscript using the Newton-Raphson method with a tolerance of 10^{-6}.

$$J_w = \frac{A\left[\pi_{D,b} exp\left(-\frac{J_w S}{\mathcal{D}}\right) - \pi_{F,b} exp\left(\frac{J_w}{k_F}\right)\right]}{1 + \frac{B}{J_w}\left[exp\left(\frac{J_w}{k_F}\right) - exp\left(-\frac{J_w S}{\mathcal{D}}\right)\right]} \tag{13}$$

$$J_s = \frac{B\left[c_{D,b} exp\left(-\frac{J_w S}{\mathcal{D}}\right) - c_{F,b} exp\left(\frac{J_w}{k_F}\right)\right]}{1 + \frac{B}{J_w}\left[exp\left(\frac{J_w}{k_F}\right) - exp\left(-\frac{J_w S}{\mathcal{D}}\right)\right]} \tag{14}$$

Using numerical integration to calculate $Q_{D(N+1)}$ given Q_{D1} we solve Eq (S3) again using the Newton-Raphson method with a tolerance of 10^{-3}.

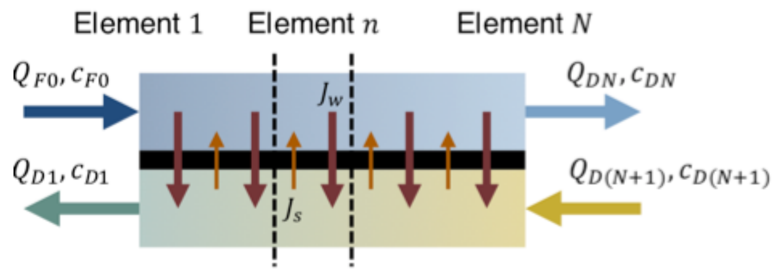

Fig. A1: Schematic of a counter-current FO membrane module of area A_m discretized into N elements. The numerical subscript n (1 to N) denotes the flow rate or concentration of the stream leaving element n.