



Data Article

Dataset of reverse osmosis membrane transport properties calculated with and without assumptions about concentration polarization and solute rejection and the errors associated with each assumption



Mikayla D. Armstrong, Riley Vickers, Orlando Coronell*

Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

ARTICLE INFO

Article history:

Received 21 July 2022

Revised 5 August 2022

Accepted 8 August 2022

Available online 12 August 2022

Keywords:

Permeance

Selectivity

Diffusive transport

Flux

Osmotic pressure

Cross-flow

Filtration

ABSTRACT

The data shared in this work represent aspects of the performance of reverse osmosis membranes during filtration. We present pressure, permeate flux, and solute rejection data gathered during cross-flow filtration experiments, which were used to (i) model water and solute permeation through the membranes and (ii) calculate concentration polarization moduli and a suite of transport properties, including water permeance, solute permeance, and water-solute selectivity. Membrane transport properties were calculated with the different approaches commonly used to simplify transport property calculations. Typical calculations of these transport properties often use simplifying assumptions (e.g., negligible concentration polarization and solute rejection close to 100%). However, the extent of the errors associated with using simplifying assumptions in this context were not previously known or quantified. This publication and corresponding dataset pertain to figures presented in the accompanying work (Armstrong et al., 2022) [1].

DOI of original article: [10.1016/j.memsci.2022.120856](https://doi.org/10.1016/j.memsci.2022.120856)

* Corresponding author.

E-mail address: coronell@unc.edu (O. Coronell).<https://doi.org/10.1016/j.dib.2022.108538>2352-3409/© 2022 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>)

Specifications Table

Subject	Water Science and Technology
Specific subject area	Formulations and calculations of reverse osmosis membrane performance properties
Type of data	Table Figure
How the data were acquired	<p>We quantified the transport properties of ESPA3 and SWC4+, two unmodified commercial membranes (Hydranautics, Oceanside, CA). The raw data was collected from cross-flow filtration experiments performed on a custom-built cross-flow filtration device.</p> <p>Pressure data was measured by electronic transducers (Omega Engineering, Swedesboro, NJ)</p> <p>Permeate flux data was measured with an electronic balance (Ohaus Adventurer, Parsippany, NJ) and a timer.</p> <p>Rejection was calculated from solute concentration data of permeate and feed samples. Sodium chloride was quantified with a conductivity probe (Fisherbrand accumet 13-620-163 and AR60 benchtop, Fisher Scientific, Pittsburgh, PA). Arsenic speciation (trivalent and pentavalent) was determined by high-performance liquid chromatography (1290 and 1260 Infinity, Agilent Technologies, Santa Clara, CA) coupled to inductively coupled mass spectrometry (7500 Series, Agilent Technologies, Santa Clara, CA). Boron was quantified by the azomethine-H colorimetric method using a spectrophotometer (HP 8452A diode array spectrophotometer, Agilent Technologies, Santa Clara, CA) and Olis Spectral Works software (v5.888.272).</p> <p>Mass transfer, advective transport, and diffusive transport coefficients were determined from the permeate flux and solute rejection data using the non-linear least-squares function (port algorithm, bounded fit, with initial guesses) in R (v4.1.3).</p> <p>Water and solute permeance were calculated from permeate flux, solute rejection, solute concentrations in the feed and permeate, pressure, and the mass transfer coefficient (i.e., using the solution-diffusion model framework). We calculated water and solute permeance with no simplifying assumptions concerning concentration polarization and rejection (termed "reference" permeance) and with three simplification scenarios, each employing varied simplifying assumptions. Percent error of the three simplification scenarios were calculated in reference to the reference membrane performance.</p>
Data format	Raw Analyzed
Description of data collection	Membranes were compacted in a cross-flow filtration system with laboratory-grade water at 33 bar for 24 h. Then filtration was performed at eight pressures (4.14–33 bar at 4.14 bar intervals) with NaCl, As(V), As(III), and boron in the feed solution. Pressure was maintained for three hours at every pressure (highest first), after which permeate flux, feed, and permeate samples were collected.
Data source location	Department of Environmental Sciences and Engineering Gillings School of Global Public Health University of North Carolina at Chapel Hill Chapel Hill, North Carolina 27599 United States
Data accessibility	<p>Repository name: Open Science Framework</p> <p>Data identification number: 10.17605/OSF.IO/PU5AJ</p> <p>Direct URL to data: https://osf.io/pu5aj/</p> <p>Instructions for accessing these data: Follow the link to the data and download the Excel file hosted in the repository.</p>
Related research article	M.D. Armstrong, R. Vickers, O. Coronell, Trends and errors in reverse osmosis membrane performance calculations stemming from test pressure and simplifying assumptions about concentration polarization and solute rejection, J. Membr. Sci. (2022) 120856. 10.1016/j.memsci.2022.120856

Value of the Data

- These data are useful to understand and estimate the errors in membrane transport properties that result from making assumptions about concentration polarization and solute rejection in water and solute permeance calculations.
- These data are useful for the determination of more accurate methods to estimate water and solute permeance in future permeation experiments.
- Membrane researchers will find these data helpful in the comparison of their datasets with those in the literature, in terms of the error associated with concentration polarization and solute rejection, as well as in the design of their cross-flow experiments.
- The membrane community will find these data important in projecting a more accurate empirical trade-off line for water-solute selectivity as a function of water permeance.
- This dataset includes the most commonly tested solute, sodium chloride, as well as other solutes relevant to reverse osmosis applications, arsenic and boron.
- Researchers will be able to quickly implement parameter fittings of mass transport coefficients to their own data by using the included methodology and pseudo code.

1. Data Description

The data provided [2] describe the cross-flow filtration conditions and transport properties of a high- and low-flux membrane (ESPA3 and SWC4+, respectively) in terms of pressure, permeate flow rate, permeate flux, solute concentrations, solute rejection, mass transfer coefficient, diffusive transport coefficient, advective transport coefficient, concentration polarization modulus (β), osmotic pressure, water permeance, solute permeance, and water-solute selectivity. Individual rows of data correspond to the applied pressure at which permeate flow rate and solute concentrations were collected during cross-flow filtration experiments (i.e., the pressure recorded in the first column of every sheet). Error was determined from the percent differences between a reference permeance value, termed “reference” water and solute permeance, and three scenario calculations of permeance. Reference water permeance was determined from the slope of the linear relationship between pressure (i.e., applied pressure minus osmotic pressure, inclusive of concentration polarization), and permeate flux using the built-in linear trendline in Excel with the intercept set to zero. Reference solute permeance was determined from the permeate flux, solute rejection data, and the mass transfer coefficient (Table 4; Sections 2.4 and 2.5). The appendix contains pseudo code in R (v.4.1.3) for the determination of the mass transfer coefficient (Sections 1.2 and 2.4). The three different scenario equations (Table 4) relate to the accounting of concentration polarization in the calculations of water and solute permeance: Scenario #1—concentration polarization was neglected ($\beta = 1$), Scenario #2—the concentration polarization modulus (β) was chosen as 1.2, and Scenario #3—concentration polarization was accounted for through the mass transfer coefficient (k). The three scenarios also use the simplifying assumption that solute rejection is equal to one to enable approximating the concentration polarization modulus to $e^{(J_p/k)}$, where J_p is permeate flux. The water-solute selectivity was calculated as the quotient of water and solute permeance. Percent error between the scenarios and the reference permeance were calculated for the water permeance, solute permeance, and water-solute selectivity.

We provided all data in one Excel file in the OSF repository called [Reference_and_simplified_membr_transport_properties_DIB.xls]. The file is split into raw data and analyzed data. Worksheets “ESPA3_1_raw,” “ESPA3_2_raw,” “SWC4_1_raw,” and “SWC4_2_raw” contain pressure, permeate flow rate, feed concentration, and permeate concentration for duplicate measurements in cross-flow filtration experiments. Worksheets “ESPA3_1_analyzed,” “ESPA3_2_analyzed,” “SWC4_1_analyzed,” “SWC4_2_analyzed,” contain permeate flux, solute rejection, feed osmotic pressure, permeate osmotic pressure, concentration polarization modulus, water permeance, solute permeance, and percent errors between scenario values and reference values for each replicate. Worksheets “ESPA3_avg_selectivity” and “SWC4_avg_selectivity”

contain the average and standard deviation (of replicates at the same condition) of pressure, permeate flux, water-solute selectivity, and percent errors between scenario selectivities and reference selectivities. The Excel worksheet names indicate if the data is raw or analyzed and each sheet has only the data of a replicate membrane, indicated with a one or two, except for “ESPA3_avg_selectivity” and “SWC4_avg_selectivity,” which contain certain averaged data of the replicates for each membrane type.

1.1. Cross-Flow Filtration Data

In the Excel file, worksheets “ESPA3_1_raw”, “ESPA3_2_raw”, “SWC4_1_raw”, and “SWC4_2_raw” contain the applied pressure (bar), permeate flow rate (g.min⁻¹), and solute concentrations of feed and permeate samples (NaCl: mS.cm⁻¹, As(V): µg.L⁻¹, As(III): µg.L⁻¹, boron: mg.L⁻¹) collected during cross-flow filtration experiments. These data were used in the calculations for permeate flux and solute rejection (see Section 2.4).

1.2. Mass Transport Parameters

The parameters in Table 1 were determined by non-linear least squares fitting (R v4.1.3, port algorithm, bounded, with initial guesses; see Appendix and Section 2.4) according to Eq. (1) using the permeate flux and solute rejection data analyzed from the raw cross-flow filtration data (Section 1.1). In this case, the mass permeation of each solute through the membrane is described as a combination of advective ($\bar{\alpha}$, dimensionless) and diffusive (\bar{B} , L.m⁻² h⁻¹) transport. The mass transfer coefficient in solution (k , L.m⁻² h⁻¹) describes the back-diffusion of solutes away from the concentration polarization layer. We used fitted mass transfer coefficients

Table 1

Advective transport coefficients ($\bar{\alpha}$), diffusive transport coefficients (\bar{B}), and mass transfer coefficients (k) of high- and low-flux membranes for each solute as defined by Eq. (1). Values are from the individual fittings of the replicates for each membrane. The first ESPA3 replicate and both SWC4 replicates were run in the same cross-flow filtration experiment and thus have the same mass transfer coefficients (see Section 2.4).

Solute	$\bar{\alpha}$ (dimensionless)	\bar{B} (L.m ⁻² h ⁻¹)	k (L.m ⁻² h ⁻¹)
High-flux membrane, ESPA3 (replicate one)			
As(V)	0.0237	0.0809	140.57
NaCl	0.0024	0.1383	220.94
As(III)	0.0000	5.5190	178.31
Boron	0.0576	19.379	174.18
High-flux membrane, ESPA3 (replicate two)			
As(V)	0.0131	0.0291	104.36
NaCl	0.0048	0.1691	164.02
As(III)	0.0213	3.2478	132.37
Boron	0.1250	11.361	129.31
Low-flux membrane, SWC4 (replicate one)			
As(V)	0.0154	0.0181	140.57
NaCl	0.0010	0.0215	220.94
As(III)	0.0000	3.3035	178.31
Boron	0.0255	2.8035	174.18
Low-flux membrane, SWC4 (replicate two)			
As(V)	0.0124	0.0454	140.57
NaCl	0.0010	0.0252	220.94
As(III)	0.0000	0.3159	178.31
Boron	0.0168	3.0755	174.18

in the calculation of concentration polarization moduli (β , dimensionless), water permeance (A , $\text{L}\cdot\text{m}^{-2}\text{ h}^{-1}\text{ bar}^{-1}$), and solute permeance (B , $\text{L}\cdot\text{m}^{-2}\text{ h}^{-1}$), which are in the Excel file. The contents of [Table 1](#) are not in the Excel file.

1.3. Actual Concentration Polarization Moduli

We provide the actual concentration polarization moduli (see [Section 2.5](#)) at every pressure for each solute during cross-flow filtration through the high- and low-flux membranes. The concentration polarization moduli (i.e., column titles of “modulus_AsV,” “modulus_AsIII,” “modulus_naCl,” “modulus_boron”) are in the “ESPA3_1_analyzed,” “ESPA3_2_analyzed,” “SWC4_1_analyzed,” and “SWC4_2_analyzed” worksheets. Concentration polarization moduli represent the extent of concentration polarization that has occurred during filtration where unity indicates no concentration polarization has occurred. The moduli were used in the calculation of osmotic pressure ([Section 2.5](#)) and reference solute permeance ([Table 4](#)).

1.4. Water Permeance

The “ESPA3_1_analyzed,” “ESPA3_2_analyzed,” “SWC4_1_analyzed,” and “SWC4_2_analyzed” worksheets contain water permeance (A) calculated according to the reference condition, “reference,” and Scenarios #1–3, as well as the intermediate quantities required to calculate water permeance; for example, osmotic pressure (π , bar; see [Section 2.5](#)) and the difference between applied pressure and osmotic pressure ($\Delta P - \Delta\pi$, bar; see [Table 4](#)).

The column names pertaining to osmotic pressures contain “pi.” The feed osmotic pressures ($\pi_{f,s}$) of each solute are in the columns, “feed_pi_AsV,” “feed_pi_AsIII,” “feed_pi_naCl,” and “feed_pi_boron.” The permeate osmotic pressures ($\pi_{p,s}$) of each solute are in the columns, “permeate_pi_AsV,” “permeate_pi_AsIII,” “permeate_pi_naCl,” and “permeate_pi_boron.” The total feed osmotic pressure (π_f) is indicated as “tot_feed_pi,” total osmotic pressure at the wall of the membrane (π_w) is indicated as “tot_membr_wall_pi,” and the total permeate osmotic pressure (π_p) is indicated as “tot_permeate_pi.” The delta osmotic pressure terms ($\Delta\pi$, bar) used in the different calculations of water permeance are called, “delta_pi_beta_1,” “delta_pi_beta_1.2,” and “delta_pi_actual_beta” referring to Scenario #1, #2, and #3, respectively, where “delta_pi_actual_beta” was also used to determine reference water permeance.

The columns pertaining to $\Delta P - \Delta\pi$ are “applied_p_minus_delta_pi_beta_1,” “applied_p_minus_pi_beta_1.2,” and “applied_p_minus_wall_pi,” referring to Scenario #1, #2, and #3, respectively, where “applied_p_minus_wall_pi” was also used to determine reference water permeance.

The names of the columns pertaining to water permeance contain an “A”: “reference_A,” “scenario1_A,” “scenario2_A,” and “scenario3_A.” Reference water permeance is a single value for all permeate fluxes and pressures. The percent errors between the scenario water permeances and the reference water permeance are in columns, “scenario1_A_error,” “scenario2_A_error,” and “scenario3_A_error.”

1.5. Solute Permeance

The “ESPA3_1_analyzed,” “ESPA3_2_analyzed,” “SWC4_1_analyzed,” and “SWC4_2_analyzed” worksheets contain solute permeance (B) data calculated according to the reference condition, “reference,” and Scenarios #1–3 (see [Table 4](#)), as well as the intermediate quantities required to calculate solute permeance: permeate flux, solute rejection, and concentration polarization modulus ([Section 2.5](#)). The mass transfer coefficient required to calculate reference solute permeance is given in [Table 1](#). The names of the columns pertaining to solute permeance contain a “B” and specify the solute, e.g., “reference_B_AsV,” “scenario1_B_AsV,” “scenario2_B_AsV,”

and “scenario3_B_AsV.” The percent errors between the scenario solute permeances and the reference solute permeances are similarly named per solute, e.g., “scenario1_B_error_AsV,” “scenario2_B_error_AsV,” and “scenario3_B_error_AsV.”

1.6. Water-Solute Selectivity

Water-solute selectivity is an averaged quantity (Section 2.5; Table 4) and is contained in worksheets, “ESPA3_avg_selectivity” and “SWC4_avg_selectivity.” These sheets have the average and standard deviation for replicate membrane samples of pressure, permeate flux, and selectivity, as well as percent errors between the scenario selectivities and reference selectivities. The column names are scenario and solute specific, e.g., “reference_selectivity_nacl,” “stdev_reference_selectivity_nacl,” “scenario1_selectivity_nacl,” “stdev_scenario_selectivity_nacl,” and “scenario1_selectivity_error_nacl.”

2. Experimental Design, Materials and Methods

2.1. Cross-Flow Filtration

Cross-flow experiments were performed with a custom-built cross-flow filtration apparatus described elsewhere [3,4]. Briefly, water was pumped from a large, temperature-controlled (22 °C) reservoir (20 L) to four pressurized cells (active membrane area: $3.557\text{E-}03\text{ m}^2$) in series at $16\text{ L}\cdot\text{h}^{-1}$ flow ($14\text{ cm}\cdot\text{s}^{-1}$ cross-flow velocity) at pH 5.3. Compaction was performed with laboratory-grade water (LGW; $\geq 17.8\text{ M}\Omega\cdot\text{cm}$, Dracor, Durham, NC) for 24 h at 33 bar. After compaction, the reservoir was spiked with a solution of sodium chloride ($\geq 99\%$, Fisher Scientific, Pittsburgh, PA), arsenous acid (+3 at $1000\text{ }\mu\text{g}/\text{mL}$ in 2% HCl, High Purity Standards, North Charleston, SC), arsenic acid (+5 at $1000\text{ }\mu\text{g}/\text{mL}$ in H_2O , High Purity Standards, North Charleston, SC), and boric acid to reach a target feed concentration of $2000\text{ mg}\cdot\text{L}^{-1}$ NaCl, $1000\text{ }\mu\text{g}\cdot\text{L}^{-1}$ H_3AsO_3 , $1000\text{ }\mu\text{g}\cdot\text{L}^{-1}$ H_3AsO_4 , and $200\text{ mg}\cdot\text{L}^{-1}$ H_3BO_3 . These concentrations were either typical of those in the literature (NaCl [5–10]) or chosen so that the permeate concentration would be greater than the detection limits of the quantification method. Filtration was performed for three hours at each of eight pressures, sequentially (33.1, 29.0, 24.8, 20.7, 16.5, 12.4, 8.27, then 4.14 bar). Duplicate permeate samples were collected for a prescribed time (30 s to 2 min, depending on the pressure) at the end of the three hours and weighed, resulting in permeate flow rate measurements. Then, permeate samples (14 mL total, 2 mL for arsenic quantification and 5 mL for sodium chloride and boric acid quantification) were collected in duplicate, in metal-free tubes. During permeate collection, samples of the feed (14 mL total) were collected and used for the solute rejection calculations.

2.2. Membranes

Membranes used were a brackish water membrane, ESPA3, and a seawater membrane, SWC4+ (Hydranautics, Oceanside, CA). The data provided here and in the Excel file represent unmodified membranes. Prior to use, the membranes were rinsed with LGW and stored submerged in 2 L of LGW at 4 °C for three days.

2.3. Solute Quantification

Sodium chloride. The conductivity of the permeate and feed samples were measured with a Fisherbrand™ accumet™ Four-Cell Conductivity/ATC Probe and an accumet™ XL60 benchtop

meter purchased from Fisher Scientific (Pittsburgh, PA). The permeate samples were measured neat and the feed samples were diluted with LGW to fit a linear range of 0.04–5.2 mS.cm⁻¹. Reported conductivities were adjusted by their dilution factor. Individual standard curves were made for the feed and permeate samples to determine the molar concentration of the samples for osmotic pressure calculations. The equation of the standard curve was $c_{molar} = 0.0832c_{cond} - 4.00E-05$ ($R^2 = 0.9999$) for the permeate samples and $c_{molar} = 0.0988c_{cond} - 0.0013$ ($R^2 = 0.9992$) for the feed samples, where c_{molar} is NaCl concentration (M) and c_{cond} is the measured conductivity (S.m⁻¹).

Boric acid. The mass of boric acid in the feed and permeate samples were determined by an azomethine-H spectroscopic method (420 nm, 1 cm cuvette) reported elsewhere [3] using a Hewlett Packard diode array spectrometer and metal-free containers. The feed and permeate samples were diluted with LGW to fit a linear range of 0.2–6 mg.L⁻¹. A standard curve was made on the day of analysis for all samples.

Arsenic. The As(III) and As(V) species of the feed and permeate samples were quantified by high-performance liquid chromatography (HPLC) coupled to inductively coupled plasma mass spectrometry (ICP-MS) using an ammonium carbonate mobile phase (60 mM, 1% EtOH, pH 9 [11]). The permeate samples were quantified neat; the feed samples and standards were diluted with 0.1 M ammonium acetate (pH 5.75). The linear range of the standard curves was 1–500 ppb. The limits of detection (quantification) were 4.8 ppb (14.5 ppb) and 3.6 ppb (10.9 ppb) for As(III) and As(V), respectively. If a sample measurement was below the LOD, we reported half of the LOQ. If measurements were below the LOQ and above the LOD, we reported the LOQ. For quality control, one sample was quantified a second time every twelve samples as well as the lowest standard and a trace metals in drinking water standard (26 component trace metals in drinking water, in 2% HNO₃ + Tr HF, Mix A, High Purity Standards, North Charleston, SC).

2.4. Parameter Fitting

We determined the mass transfer coefficient (k , L.m⁻² h⁻¹), solute diffusive transport coefficient (\bar{B} , L.m⁻² h⁻¹) and advective transport coefficient ($\bar{\alpha}$, dimensionless) by fitting these parameters to permeate flux (J_v , L.m⁻² h⁻¹) and solute rejection (R , dimensionless) data according to

$$R = \frac{(1 - \bar{\alpha})J_v}{(\bar{B} + \bar{\alpha}J_v)e^{(J_v/k)} + (1 - \bar{\alpha})J_v} \quad (1)$$

Each parameter had a lower and upper bound. We calculated the bounds of the mass transfer coefficient using four Sherwood correlations [12–15]; the lowest value was rounded down to the nearest integer and highest value was rounded up to the nearest integer plus one and used as the lower and upper bounds, respectively (see Tables 2 and 3).

The lower bound of the solute diffusive transport coefficient (L.m⁻² h⁻¹) was zero and the upper bound was estimated as:

$$\bar{B}_{upper\ bound} = 2 \times \frac{J_v(1 - R)}{R}. \quad (2)$$

Finally, the advective transport coefficient was bound by zero and 0.2 (dimensionless). The mass transfer coefficient (k) was determined first for As(V) (for each individual cross-flow experiment) because As(V) had the most CP of the solutes, as determined by plots of $1/J_v$ vs. $c_p/(c_f - c_p)$. Then, k was calculated for NaCl, As(III), and boron according to [17]

$$k_s = k_{As(V)} \left(\frac{D_s}{D_{As(V)}} \right)^{2/3}, \quad (3)$$

in which k and D are the mass transfer coefficient and diffusion coefficient in solution, respectively, and the subscript s refers to solutes other than As(V). The diffusion coefficients of NaCl, As(III), and boron are 1.6×10^{-9} [18], 1.16×10^{-9} [16], and 1.12×10^{-9} m² s⁻¹ [19], respectively.

Table 2

Operating conditions and constants needed for the calculation of Sherwood numbers for the calculation of the mass transfer coefficient bounds in the model fitting.

Quantity	Value	Units
Temperature	22	°C
Target flow rate	16	L.h ⁻¹
Cell channel height	8.128E-04	m
Cell channel length	3.800E-02	m
Cross-flow velocity	1.439E-01	m.s ⁻¹
Hydraulic diameter (d_H) [13]	1.592E-03	m
Density of water (ρ)	997.776	kg.m ⁻³
Dynamic viscosity of water (μ)	9.532E-04	kg.m ⁻¹ s ⁻¹
Reynolds number (Re)	240.1	dimensionless
Diffusion coefficient of As(V) (D) [16]	8.120E-10	m ² s ⁻¹
Schmidt number (Sc)	1174	dimensionless

Table 3

Sherwood numbers and mass transfer coefficients (k) used to determine the upper and lower bounds in the model fitting.

Sherwood number (dimensionless)	Mass transfer coefficient (m.d ⁻¹)	Bounds
40.84 [13]	1.800	1–6 m.d ⁻¹
42.16 [14]	1.858	41–
108.56 [15]	4.786	250 L.m ⁻² h ⁻¹
N/A	4.236 [12]	

We performed the cross-flow filtration experiments of ESPA3_1, SWC4_1, and SWC4_2 simultaneously (i.e., in three pressurized cells of the custom-built cross-flow filtration apparatus) and that of ESPA3_2 on a subsequent day. Since the mass transfer phenomena in the feed solution for different membranes run simultaneously in identical cells in one system should be the same, the mass transfer coefficients for each solute were determined as described for ESPA3_1 first and those same mass transfer coefficients were used as known constants in the fittings for SWC4_1 and SWC4_2.

The parameters were fit using the non-linear least squares function in R (v4.0.5) using the port algorithm, bounding the parameters with an upper and lower bound (as described above in this section), and providing initial guesses for each parameter. The initial guesses were the lower bound value for the mass transfer coefficient where applicable, and as follows for the advective transport coefficient (diffusive transport coefficient): 0.001 (0.01), 0.0001 (0.001), 0.001 (0.01), and 0.001 (0.01) for As(V), NaCl, As(III), and boron, respectively. Pseudo code for the parameter fittings is in the Appendix. Example fittings are shown in Fig. 1.

2.5. Calculations

In the data file provided in the data repository, we provided the raw data from each experiment, which includes pressure, permeate flow rate, and solute concentrations in the feed and permeate samples. These data were used to calculate the permeate flux, solute rejection, and osmotic pressures of the system. Permeate flux (J_v , L.m⁻² h⁻¹) was calculated as

$$J_v = \frac{\dot{m}}{a\rho}, \quad (4)$$

with \dot{m} as permeate flow rate (g.min⁻¹), a as the active membrane area (3.557×10^{-3} m²), and ρ as density of water at 22 °C (997.76 g.L⁻¹). Eq. (4) excludes necessary unit conversions. Solute rejection (R) was calculated as

$$R = \frac{c_f - c_p}{c_f} \times 100\%, \quad (5)$$

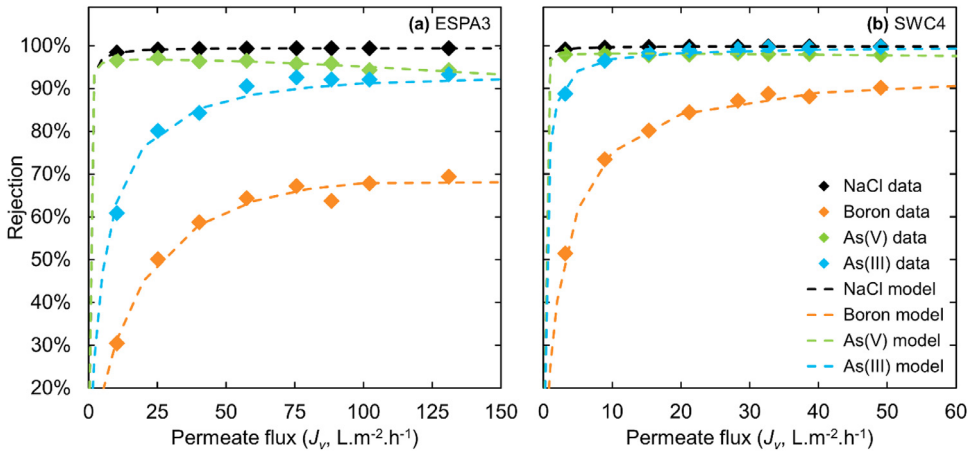


Fig. 1. Example parameter fittings (dashed lines) for the solutes rejected by a) ESPA3 and b) SWC4+ in cross-flow experiments. Markers are data corresponding to ESPA3_1 and SWC4_1. Associated parameters are in Table 1.

where c_f and c_p represent mass concentration for arsenous acid, arsenic acid, and boric acid or conductivity for sodium chloride. Osmotic pressure was estimated with the van't Hoff equation [20],

$$\pi = iCR_uT, \quad (6)$$

where i refers to the number of dissociated species in the molecule, C is the concentration of solute (M), R_u is the universal gas constant ($\text{L}\cdot\text{bar}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) and T is temperature (K). The concentrations of our samples were in the linear range for an accurate estimation of osmotic pressure from the van't Hoff approximation [20].

The concentration polarization modulus (β , dimensionless) for each solute at each pressure was calculated according to [20]

$$\beta = (1 - R) + e^{(J_v/k)}R. \quad (7)$$

Several osmotic pressure terms (bar) were calculated and used depending on the scenario. The total feed and permeate osmotic pressures (π_f and π_p , respectively) were calculated as the sums of the solute-specific feed and permeate osmotic pressures ($\pi_{f,s}$ and $\pi_{p,s}$, respectively), given as

$$\pi_f = \sum \pi_{f,s} \quad (8)$$

and

$$\pi_p = \sum \pi_{p,s}. \quad (9)$$

The total osmotic pressure at the wall of the membrane (π_w , bar) was calculated using the concentration polarization moduli of each solute (β_s , dimensionless) according to

$$\pi_w = \sum_s \beta_s \pi_{f,s}. \quad (10)$$

Table 4 contains the equations used to calculate the reference membrane transport properties, the permeance equations for Scenarios #1–3, and the corresponding water-solute selectivity. The water-solute selectivity values were calculated as the quotient between the average water and solute permeance for each respective scenario. The standard deviations of duplicate samples were calculated with the standard deviation of the population function in Excel. For water-solute selectivity, the standard deviation ($\sigma_{A_{avg}/B_{avg}}$) was calculated by propagating standard deviation

Table 4

Water permeance, solute permeance, and water-solute selectivity equations for each simplification scenario.

	Water permeance, A (L.m ⁻² h ⁻¹ .bar ⁻¹)	Solute permeance, B (L.m ⁻² h ⁻¹)	Water-solute selectivity, A/B (bar ⁻¹)
Reference	Slope of J_v vs. $[\Delta P - (\pi_w - \pi_p)]^\S$	$B = \frac{J_v(1-R)}{e^{(J_v/k)R}}$	
#1	$A = \frac{J_v}{\Delta P - (\pi_f - \pi_p)}$	$B = \frac{J_v(1-R)}{R}$	$A/B = \frac{A_{avg}}{B_{avg}}$
#2	$A = \frac{J_v}{\Delta P - (1.2\pi_f - \pi_p)}$	$B = \frac{J_v(1-R)}{1.2R}$	
#3	$A = \frac{J_v}{\Delta P - (\pi_w - \pi_p)}$	$B = \frac{J_v(1-R)}{\beta R}$	

§ With the intercept set to zero.

from water and solute permeance as

$$\sigma_{A_{avg}/B_{avg}} = \frac{A_{avg}}{B_{avg}} \sqrt{(\sigma_{A_{avg}}/A_{avg})^2 + (\sigma_{B_{avg}}/B_{avg})^2}, \quad (11)$$

where A_{avg} and B_{avg} are the average water and solute permeance, respectively, and $\sigma_{A_{avg}}$ and $\sigma_{B_{avg}}$ are the standard error of the average water and solute permeance, respectively.

The percent error values were calculated as

$$\text{Percent error} = \frac{P_{\text{scenario}} - P_{\text{actual}}}{P_{\text{actual}}} \times 100\%, \quad (12)$$

where P is the water permeance (L.m⁻² h⁻¹.bar⁻¹), solute permeance (L.m⁻² h⁻¹), or performance in terms of water-solute selectivity (bar⁻¹), and the subscript specifies either the scenario permeance values or the reference permeance as defined in Table 4. For water and solute permeance, percent errors were calculated for individual data points and then averaged with an associated standard deviation. For water-solute selectivity, percent error was calculated from the average quantity and therefore, has no associated standard deviation.

Ethics Statement

This work did not include human subjects, animal experiments, nor data collected from social media platforms. The authors adhered to all ethics and publishing standards.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. The authors declare the following financial interests/personal relationships which may be considered as potential competing interests.

Data Availability

Dataset of reverse osmosis membrane transport properties calculated with and without assumptions about concentration polarization and solute rejection and the errors associated with each assumption (Original data) (ORNL-DAAC).

CRedit Author Statement

Mikayla D. Armstrong: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization; **Riley Vickers:** Conceptualization, Validation, Writing – review & editing; **Orlando Coronell:** Conceptualization, Methodology, Writing – review & editing, Supervision, Funding acquisition.

Acknowledgments

This work was funded in part by the [National Institute of Environmental Health Sciences](#) [Grant Nos. [P42ES031007](#) and [T32ES007018](#)], the US [National Science Foundation](#) (NSF) Graduate Research Fellowship Program Grant No. [DGE-1650115](#), and the Caroline H. and Thomas S. Royster Fellowship at UNC. The authors would like to thank Hydranautics for donating membrane materials. We sincerely thank Pete Cable for help with the arsenic speciation performed at the UNC Chapel Hill Biomarker Mass Spectroscopy Facility.

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