Solution Domain Task 1: Species Balance

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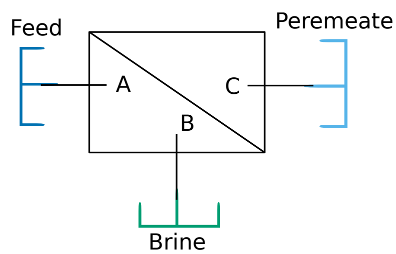
1 Problem to Solve

This looks to build off the idea presented in the custom TL domain tutorial, but also accounts for species balance. This will allow for modeling brine. Additionally, this problem aims to measure the density of the solution, accounting for the solute in the calculation. Here is a schematic of the problem:



For this problem, I will start by assuming no volume in the membrane. This means that we use a mass balance approach. If we assumed volume in the membrane component, there would be an additional set of states required to track the composition of the fluid in the membrane component, which would add a couple of equations. I'll note them at the end.

1.1 Variables

Variables are defined in the table below:

Variable	Symbol	Type	Units
Concentration	x	State Variable	kg/m^3
Pressure	P	Reservoir Parameter	Pa
Temperature	T	Reservoir Parameter	K

Variable	Symbol	Type	Units
Flow Rate	Q	State Variable	m^3/s
Density	ρ	Intermediate Variable	kg/m^3
Membrane Permeability	A_w	Membrane Parameter (TLU later)	$m^3/(N{\cdot}s)$
Solute Transport Parameter	B_s	Membrane Parameter (TLU later)	m/s
Membrane Area	A_m	Membrane Parameter	m^2
Brine Resistance	R_B	Membrane Parameter	$Pa{\cdot}s/m^3$
Osmotic Pressure	π	Intermediate Variable	Pa
Ion count	i	Fluid Parameter	-
Solute molar mass	M	Fluid Parameter	kg/mol
Density of Water	ρ_w	Fluid TLU	kg/m^3
Ideal Gas Constant	R	Fluid Property?	$J/(mol{\cdot}K)$

Subscript A refers to the feed, B refers to the brine, and C refers to the permeate.

1.2 Assumptions

We assume that the system is at steady state, that the mixing is perfect, and no gradient of salt concentration. We assume we know the concentration of the feed (x_A).

2 Equations

2.1 Density Calculation

The density for each fluid is defined as:

$$\rho = \rho_w(T, P) + x$$

This allows us to calculate the density of the solution, provided we have 3 state variables: temperature, pressure, and concentration. Density probably makes most sense as an intermediate variable, so I won't include it in my equation and variable count.

2.2 Species Conservation

The governing mass flow balance equation is shown below:

$$\rho_A Q_A + \rho_A Q_B + \rho_A Q_C = 0$$

we show how we can calculate the density as an intermediate variable in the density calculation above, so those can be excluded from the variable count. This leaves us with 3 unknowns: Q_A, Q_B, and Q_C.

The governing solute flow balance equation is shown below:

$$x_A Q_A + x_B Q_B + x_C Q_C = 0$$

This ensures that the mass of the solute is conserved in addition to the entire solution mass. When combined with the total mass balance equation earlier it ensures that the mass of the solvent is conserved as well, so a separate solvent mass balance equation is not needed. It also leaves us with 2 more unknowns: x_B and x_C, remember we assume we know x_A.

2.3 Membrane Equations

The governing membrane transport equations are shown below:

$$A_w A_m \big((P_C - P_A) - (\pi_C - \pi_A)\big) + Q_c = 0$$

$$B_s A_m \big(x_A - x_C\big) + Q_c x_C = 0$$

The first equation describes the solvent transport through the membrane, while the second describes the solute transport through the membrane. Both equations require the osmotic pressure of the feed and permeate, which we can calculate as follows:

$$\pi = i \frac{x}{M} RT$$

Osmotic pressure will be defined as an intermediate variable, so we won't include it in the variable count. In this problem we assume we know the pressures P_A and P_C. So no new variables are introduced by these equations.

2.4 Brine Resistance

At this point we have 5 unknowns, Q_A, Q_B, Q_C, x_B, and x_C, but only 4 equations (total mass balance, solute mass balance, solvent transport, and solute transport). The final required equation is the brine side pressure balance equation. Without some sort of resistance to flow on the brine side, there would be no flow through the membrane. Plus it would cause solver issues then if P_A and P_B were inequal. This pressure balance equation related to the brine side resistance is shown below:

$$P_A - P_B + Q_B R_B = 0$$

With this equation, we now have 5 equations and 5 unknowns, so we can solve the system.

3 Implementation Plan

3.1 Domain Parameters

For a given fluid, the user would need to define the following parameters:

Parameter	Symbol
Density of Solvent Table	ρ_w
Ion Count	i
Solute Molar Mass	M
Ideal Gas Constant	R

3.2 Membrane Parameters

For a given membrane, the user would need to define the following parameters:

Parameter	Symbol
Water Permeability	A_w
Solute Permeability	B_s
Membrane Area	A_m

3.3 Node Variables

We have three nodes: feed, brine, and permeate, and each node will have the following variables:

Variable	Symbol
Concentration	x
Pressure	P
Temperature	T
Flow Rate	Q

3.4 Intermediate Variables

I'm less confident here, but my first instinct would be to set these as intermediate variables:

Variable	Symbol
Osmotic Pressure	π
Density	ρ

4 What if we assume volume in the membrane?

If we assume volume in the membrane, we need to find 2 new variables, the pressure in the membrane (P_I) and the concentration of the solute in the membrane (x_I). The mass balance equations would then be modified to look like this:

$$\rho_A Q_A + \rho_A Q_B + \rho_A Q_C + \dot{\rho}_I V_I = 0$$

$$x_A Q_A + x_B Q_B + x_C Q_C + \dot{x}_I = 0$$

where V_I represents the volume in the membrane. I believe then to help reduce the number of unknowns we would set P_I to P_A. Similar logic here to the brine resistance, except instead of adding a resistance, I'm just assuming the pressure is equal for simplicity. We could easily have a resistance though, which would just add another resistance style pressure balance equation.

This still leaves us with 6 unknowns: Q_A, Q_B, Q_C, x_B, x_C, and x_I, but still only 5 equations.