Solution Domain Task 1: Species Balance

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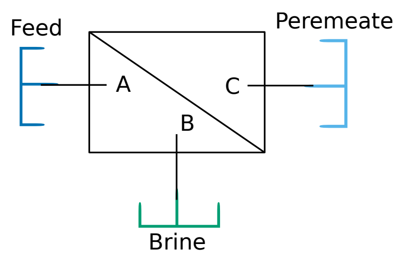
1 Problem to Solve

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
Solute Flow Rate	$\dot{m}_w$	Through Variable	kg/s
Solvent Flow Rate	$\dot{m}_x$	Through Variable	kg/s
Energy Flux	Φ	Through Variable	W
Density	ρ	Intermediate Variable	kg/m³
Membrane Permeability	A_w	Membrane Parameter (TLU later)	m³/(N·s)
Solute Transport Parameter	B_s	Membrane Parameter (TLU later)	m/s
Membrane Area	A_m	Membrane Parameter	m²
Brine Resistance	R_B	Membrane Parameter	Pa·s/m³
Osmotic Pressure	π	Intermediate Variable	Pa
Ion count	i	Fluid Parameter	-
Solute molar mass	M	Fluid Parameter	kg/mol
Density of Water	$\rho_w(T, P)$	Fluid TLU	kg/m³
Ideal Gas Constant	R	Fluid Property?	J/(mol·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.

2.2 Species Conservation

The governing solvent mass flow balance equation is shown below:

$$\dot{m}_{w,A} + \dot{m}_{w,B} + \dot{m}_{w,C} = 0$$

This leaves us with 3 unknowns: $\dot{m}_{w,A}$, $\dot{m}_{w,B}$, and $\dot{m}_{w,C}$.

The governing solute flow balance equation is shown below:

$$\dot{m}_{x,A} + \dot{m}_{x,B} + \dot{m}_{x,C} = 0$$

This ensures that the mass of the solute is conserved in addition to the entire solution mass.

2.3 Membrane Equations

The governing membrane transport equations are shown below:

$$A_w A_m \big((P_C - P_A) - (\pi_C - \pi_A) \big) + \frac{\dot{m}_{w,C}}{\rho_w(T, P_C)} = 0$$

$$B_s A_m \big(x_A - x_C \big) + \dot{m}_{x,C} = 0$$

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:

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

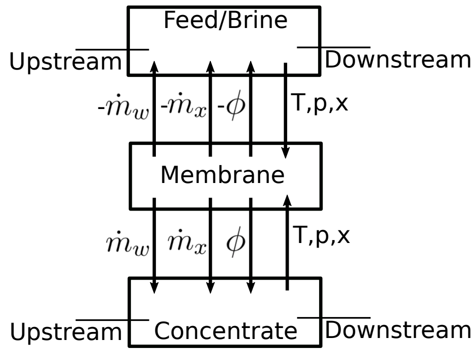
2.4 Brine Resistance

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:

$$P_A - P_B + \frac{\dot{m}_{x,B}}{\rho_w(T, P_B)} R_B = 0$$

3 Implementation Plan

The plan for modeling a segment of the membrane is shown below:



The membrane will take in inputs about the state of the two tanks and use the equations described earlier to calculate the mass flow rates of the water and solute through the membrane. Note that the brine resistance will be applied on the downstream side of the feed/brine tank, and is a separate component from the membrane.

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 Inputs

We need three state variables from each tank, described in the table below:

Variable	Symbol
Concentration	x
Pressure	P
Temperature	T

3.4 Outputs

The outputs are the mass flow rates of the water and solute through the membrane, as well as the energy flux through the membrane. The outputs are described in the table below:

Variable	Symbol
Water Flow Rate	$\dot{m}_w$
Solute Flow Rate	$\dot{m}_x$
Energy Flux	Φ

There are two sets of outputs, one for the feed side, and one for the permeate side. The feed and permeate sides are the same magnitude, but opposite sign to conserve mass and energy.

3.5 Intermediate Variables

These will be intermediate variables:

Variable	Symbol
Osmotic Pressure	π
Density of Water	ρ_w

3.6 Equations

We need an equation for each output variable. We will use the membrane transport equations to calculate $\dot{m}_w$ and $\dot{m}_x$ on the permeate side. The feed side will be the same magnitude, but opposite sign. The energy flux can be calculated as follows:

$$\Phi = \dot{m} c_p T$$

where c_p is the specific heat capacity of the solution. Notably, $\dot{m}$ has no subscript, and ideally it accounts for the mass flow rate of both the water and solute. Additionally, the specific heat capacity, c_p, of the solution should ideally be determined for the specific solution, but for now we will assume it is not a function of the concentration. Again, the equation shown above was for the permeate side, and the feed side will be the same magnitude, but opposite sign.