Independent Study

final report

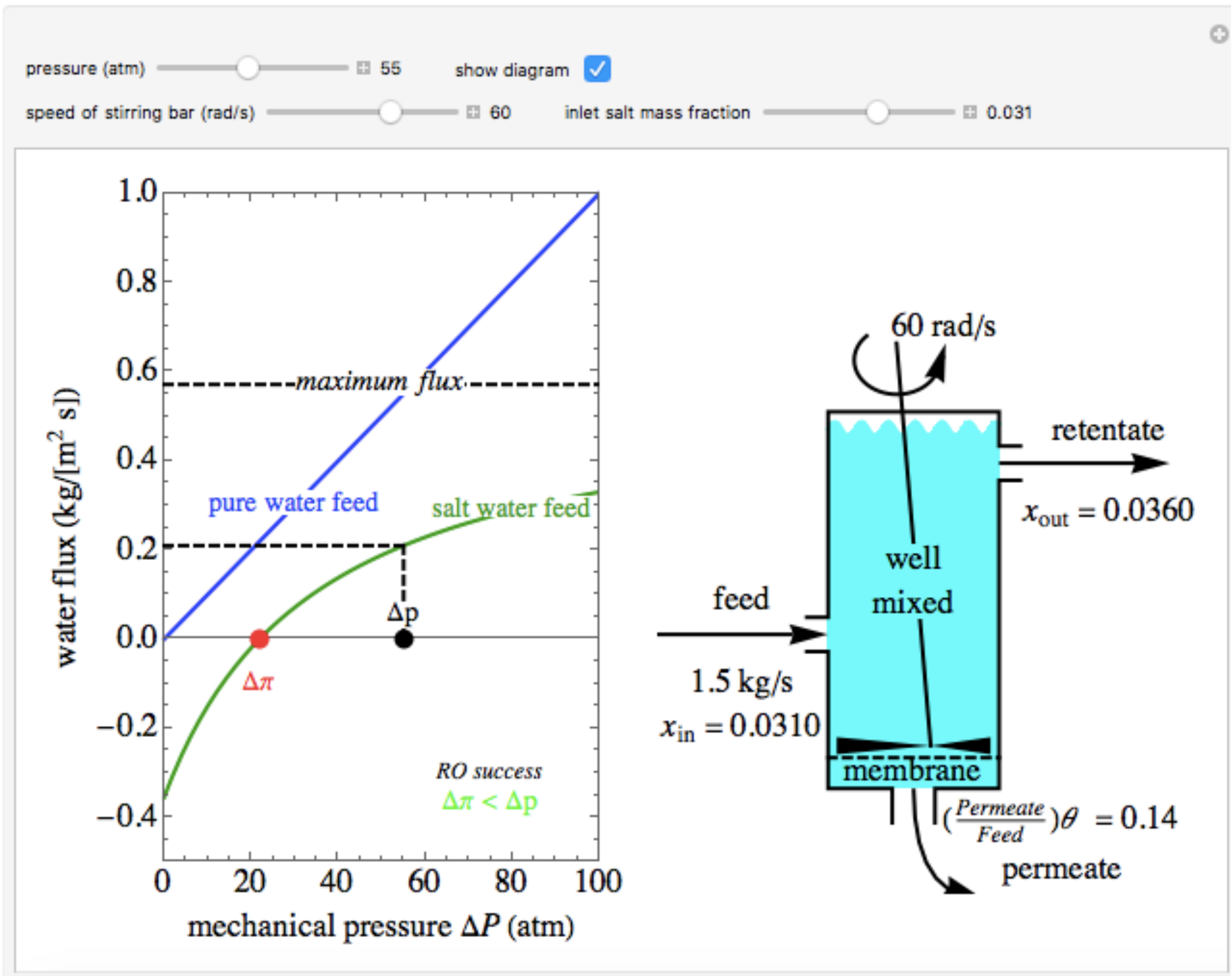
prepared for : John L. Falconer

Muqbil Alkhalaf

Summer 2017

First Simulation

Reverse Osmosis



Reverse osmosis is a separation process used to further concentrate a feed stream by overcoming the osmotic pressure with a larger mechanical pressure drop.

In this simulation we aim to help the user further investigate the dependencies and the affects of changing of pressure, inlet feed salt concentration and stirring speed on the solvent flux in a reverse osmosis process. The system has a constant temperature and inlet feed stream flow rate. The user is given control over the pressure, speed of the stirring bar, and inlet salt mass fraction with sliders.

Equations used :

First, solve for the mass transfer coefficient using the following equation:

$$\boxed{k = 0.04433\left(\frac{\omega d}{v}\right)^{0.75} \mathrm{Sc}^{0.33}\ \frac{D_{AB}}{d},}$$

where k is the mass transfer coefficient, **ω** is the rotational speed of the stirring bar (rad/s), d is the tank diameter (m), v is kinematic viscosity (m^^{2}/s), Sc is the Schmidt number (dimensionless), and D_{AB} is the diffusivity of the solute in water (m^^{2}/s).

$$\boxed{J - J_{max} = \ln 10\ k\ \rho_l}$$

Then solve for the maximum solvent flux:
where J_{max} is maximum water flux through the membrane (g/m^^{2}/s), and ρ is the density of water (g/m^^{3}).

Solve for the solvent flux:

$$\boxed{J' = \frac{J'_{max}\,(\Delta P - \Delta\pi)}{(\Delta P - \Delta\pi) + J'\ \frac{t}{K'}}}$$

where ΔP is mechanical pressure (atm), Δπ is osmotic pressure (atm), and K'/t is permeability of the membrane to the solvent (g/[atm s m^2]).

A material balance is done for salt across the system to get the value for the mass fraction of salt in the outlet stream, which is the same as the retentate mass fraction

$$\boxed{x_R = x_{out} = \frac{F'_{in}\, x_{in}}{F'_{in} - J'\, A},}$$

inside the tank (given the tank is well-mixed):

where F' is inlet feed (kg/s), X is the mass fraction of salt in the inlet stream, and A is the area of the membrane (m^2).

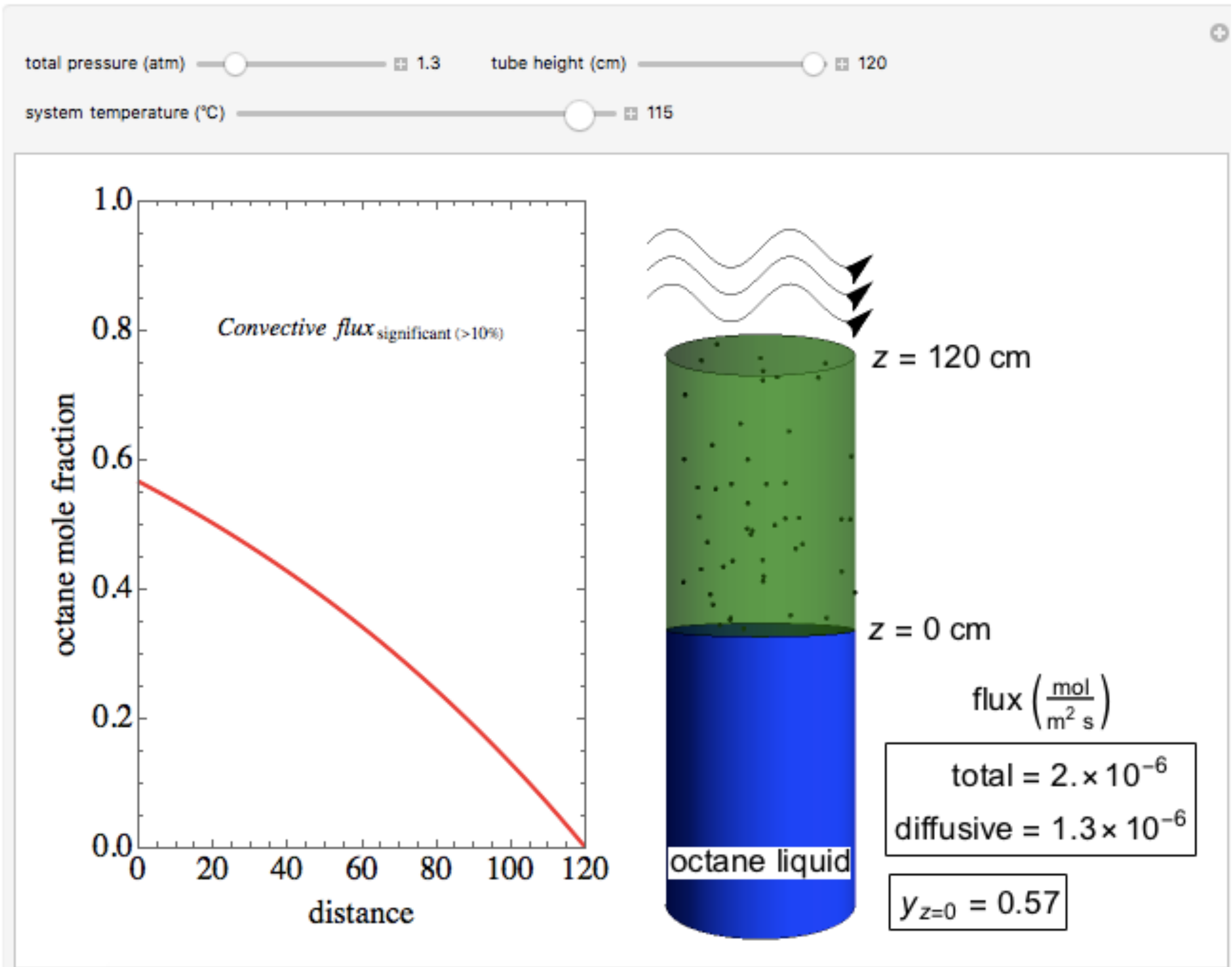
To find how much of the feed exits as the permeate , overall mass balance gives:

$$\boxed{\left(\frac{\text{Permeate}}{\text{Feed}}\right) = \theta = \frac{J'\, A}{F'_{in}},}$$

where ϴ is the fraction of the feed that is purified and exits as the permeate(i.e. cut'ϴ')[unit less]

Second Simulation

Steady State Binary Fickian Diffusion



This simulation illustrates the concentration profile and the flux in steady-state diffusion. Pure liquid octane is at the bottom of the long vertical tube, above the liquid is a quiescent layer of air. At the open end on top, air is blown to sweep the octane vapor making it's concentration at the top equal to zero.

Equations Used:

The total flux is equal to the diffusive flux plus the convective flux:

$$J_{\text{diff}} = \frac{C_m D_{AB} P^{sat}}{L P},$$
$$J_{\text{tot}} = D_{AB} \frac{C_m}{L} \ln\left(\frac{1}{1-P^{sat}/P}\right),$$

where J_{diff} is the diffusive flux (mol/[m^2 s]), Subscript J_{tot} is the total flux (mol/[m^2 s]), Cm is total concentration (mol/m^3), D_{AB} is diffusivity (cm^2/s), P^{sat} vapor pressure (atm), L is the tube height (cm), and P is total pressure (atm).

The saturation pressure is found using the Antoine equation:

$$P^{sat} = 10^\wedge\left(A - \frac{B}{T+C}\right),$$

where A, B, and C are Antoine constants, and T is temperature (C^{o}).

If the diffusive flux dominates (greater than 90% of total flux), we assume that the convective flux is zero, the concentration profile is:

$$y = -\frac{z P^{sat}}{L P} + \frac{P^{sat}}{P},$$

where z is tube height (cm).

When the convective flux becomes significant (less than 10% of total flux), the concentration profile is:

$$y = 1 - \left(\frac{1-y_{A,L}}{1-y_{A,0}}\right)^{z/L} (1 - y_{A,0}),$$

where $Y_{A,L}$ is mole fraction at z=L, and $Y_{A,0}$ is mole fraction at z=0.