CM3120: Module 3

Diffusion and Mass Transfer I

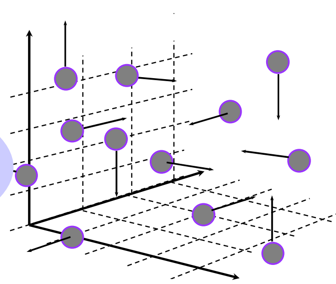
I. Introduction to diffusion/mass transfer
II. Classic diffusion and mass transfer—Quick Start a): 1D Evaporation
III. Classic diffusion and mass transfer—Quick Start b): 1D Radial droplet
IV. Cycle back: Fick's mass transport law
V. Microscopic species A mass balance
VI. Classic diffusion and mass transfer—c): 1D Mass transfer with chemical reaction

CM3120: Module 3

Module 3 Lecture II

Quick Start 1:

1D Evaporation



Professor Faith A. Morrison
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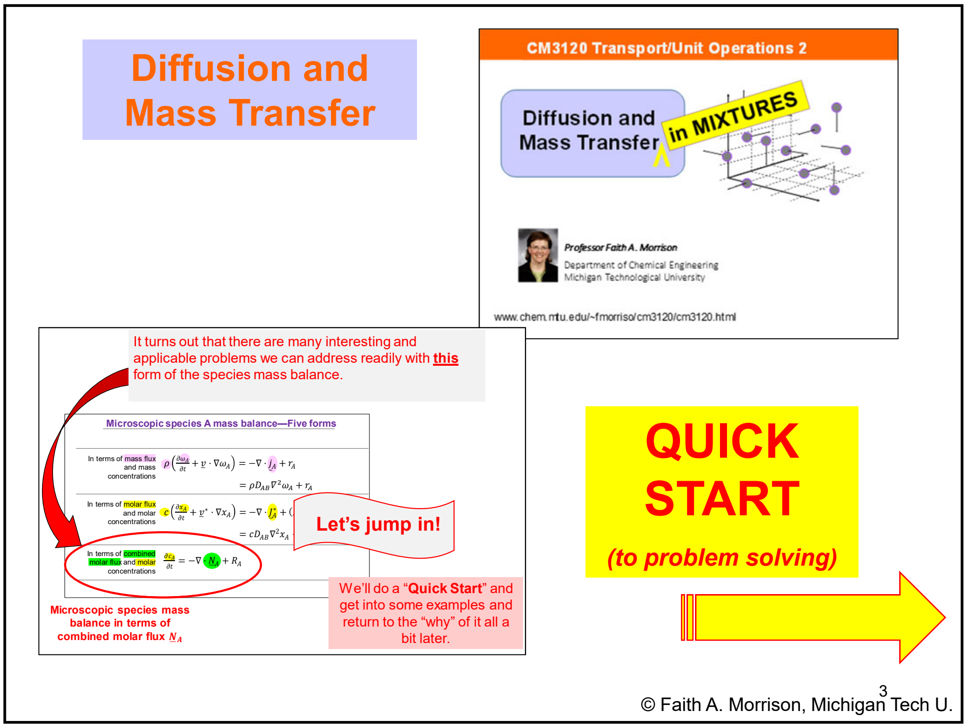
Michigan Technological University

www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html



It turns out that there are many interesting and applicable problems we can address readily with **this** form of the species mass balance.

Microscopic species A mass balance—Five forms

In terms of mass flux and mass concentrations

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = -\nabla\cdot\underline{j}_A + r_A$$
$$= \rho D_{AB}\nabla^2\omega_A + r_A$$

In terms of molar flux and molar concentrations

$$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^*\cdot\nabla x_A\right) = -\nabla\cdot\underline{J}_A^* + ($$
$$= cD_{AB}\nabla^2 x_A$$

In terms of combined molar flux and molar concentrations

$$\frac{\partial c_A}{\partial t} = -\nabla\cdot\underline{N}_A + R_A$$

Let's jump in!

Microscopic species mass balance in terms of combined molar flux $\underline{N}_A$

We'll do a "**Quick Start**" and get into some examples and return to the "why" of it all a bit later.

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Diffusion and Mass Transfer QUICK START

Using the **microscopic species mass balance** in terms of combined molar flux and molar concentrations

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

QUICK START

$c_A [=] \frac{moles\ A}{volume\ mix} = x_A c =$ the concentration of A in the mixture

$\underline{N}_A [=] \frac{moles\ A}{area \cdot time} =$ combined molar flux of A (both diffusion and convection) relative to stationary coordinates

$R_A [=] \frac{moles\ A}{volume\ mix \cdot time} =$ rate of production of A by reaction per unit volume mixture

$c [=] \frac{moles\ mix}{volume\ mix} =$ molar density of the mixture (for ideal gases $c = \frac{n}{V} = \frac{P}{RT}$)

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Diffusion and Mass Transfer QUICK START

Combined molar flux:

$$\underline{N}_A = \begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz}$$

QUICK START

$\underline{N}_A [=] \frac{moles\ A}{area \cdot time}$

combined molar flux of A

(due to both diffusion and convection)

Flux of moles of species A, both magnitude and direction, in the mixture

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Diffusion and Mass Transfer QUICK START

Using **Fick's law of diffusion** in terms of the same combined molar flux:

$$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$$

QUICK START

$\underline{N}_A [=] \frac{moles\ A}{area \cdot time}$ = combined molar flux of A (both diffusion and convection) relative to stationary coordinates

$x_A [=] \frac{moles\ A}{moles\ mix}$ = mole fraction of A

$D_{AB} [=] \frac{cm^2}{s}$ = diffusion coefficient (diffusivity) of A in B

$c [=] \frac{moles\ mix}{volume\ mix}$ = molar density of the mixture (for ideal gases $c = \frac{n}{V} = \frac{P}{RT}$)

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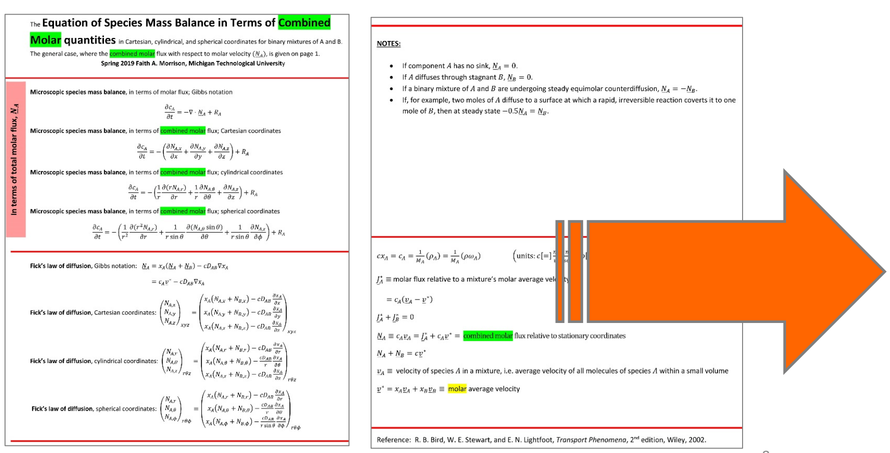
Diffusion and Mass Transfer QUICK START

Using **worksheets** to learn the common modeling assumptions

QUICK START


The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.
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In terms of total molar flux, $\underline{N}_A$

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

NOTES:

- If component A has no sink, $\underline{N}_A = 0$.
- If A diffuses through stagnant B, $\underline{N}_B = 0$.
- If a binary mixture of A and B are undergoing steady equimolar counterdiffusion, $\underline{N}_A = -\underline{N}_B$.
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction coverts it to one mole of B, then at steady state $-0.5\underline{N}_A = \underline{N}_B$.

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https://pages.mtu.edu/~fmorriso/cm3120/species_mass_bal_3_combinedmolarflux.pdf

Microscopic Species Mass Balance

QUICK START

The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

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In terms of total molar flux, $\underline{N}_A$

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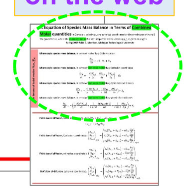
$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,z}}{\partial \phi}\right) + R_A$$

Note: this handout is on the web



pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html

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Fick's Law of Diffusion in terms of Combined Molar Flux $\underline{N}_A$

QUICK START

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

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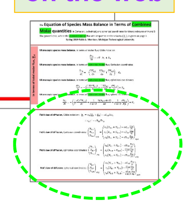

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Handy reminder of definitions and relationships among mixture quantities

QUICK START

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ $\left(\text{units: } c[=]\frac{mol\ mix}{vol\ soln}; \rho[=]\frac{mass\ mix}{vol\ soln}; c_A[=]\frac{mol\ A}{vol\ soln}; \rho_A[=]\frac{mass\ A}{vol\ soln}\right)$

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ $\left(\text{units: } \underline{J}_A^*[=]\frac{mole}{area\cdot time}\right)$

$= c_A(\underline{v}_A - \underline{v}^*)$

$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ combined molar flux relative to stationary coordinates

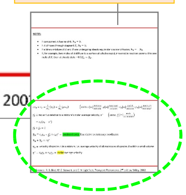
$\underline{N}_A + \underline{N}_B = c\underline{v}^*$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a sm

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 200

Note: this handout is on the web



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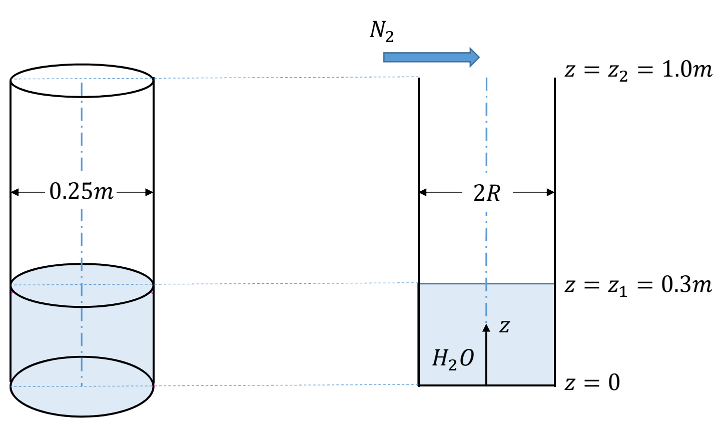
1D Evaporation from tank

QUICK START

Example 1: Water $(40^oC, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^oC, 1.0\ atm)$ from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. **What is the rate of water evaporation?**



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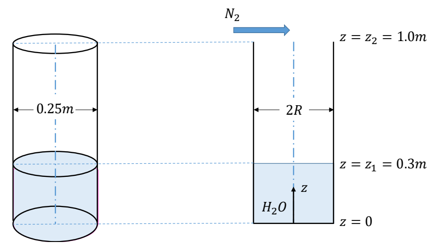
Interrogating the problem:

QUICK START

Example: Water $(40^oC, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^oC, 1.0\ atm)$ from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. **What is the rate of water evaporation?**



Why does the water evaporate?

What limits the rate of evaporation?

What could be done to accelerate the evaporation?

What could be done to slow down the evaporation?

What is the driving physics?

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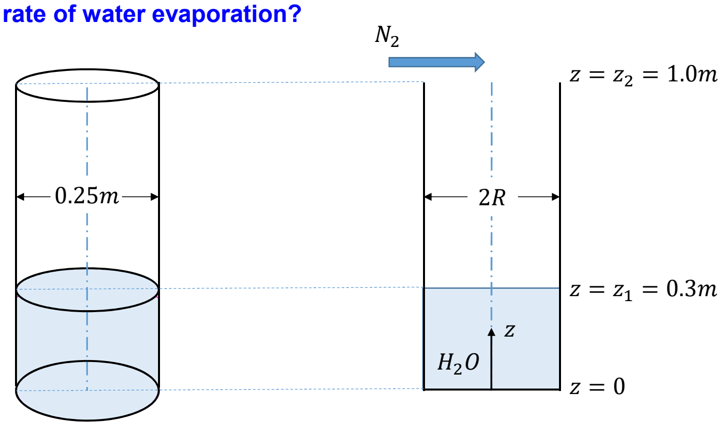
1D Evaporation from tank

QUICK START

Example 1: Water $(40^oC, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^oC, 1.0\ atm)$ from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. What is water mole fraction as a function of vertical position in the tank? You may assume ideal gas properties. **What is the rate of water evaporation?**



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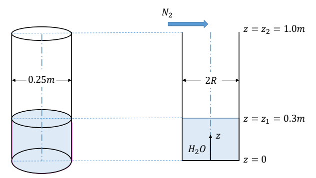
1D Evaporation from tank

QUICK START

Example: Water $(40^o C, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^o C, 1.0\ atm)$ from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. **What is the rate of water evaporation?**



Solve.

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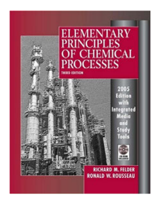
Raoult's Law

*Reference: **Felder and Rousseau**, 3rd Edition, Section 6.3, Gas-Liquid Systems, One Condensable Component*



"A law that describes the behavior of gas-liquid systems over a wide range of conditions provides the desired relationship [between $T, P,$ and y_A]. If a gas at temperature T and pressure P contains a saturated vapor whose mole fraction is y_A (mole vapor/mol total gas), and if this vapor is the only species that would condense if the temperature were slightly lowered, then the partial pressure of the vapor in the gas equals the pure-component vapor pressure $p_A^*(T)$ at the system temperature, [which we look up from tables or data correlations].

Raoult's Law (single condensable component)

$$p_A = y_A P = p_A^*(T)$$

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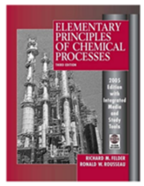
Revisiting and using important concepts/physics

Pre-reqs

Where are we now?

Michigan Tech

CM2110



CM2120

Summary

CM2110

1. Steady mass balances
2. Steady energy balances (how to calc. energy)
3. ~~MEB-Mechanical Energy Balance~~ (no friction)
4. Phase equilibria (Raoult's Law)

CM2120/CM3215

1. MEB-Mechanical Energy Balance (with friction)
2. Pumps
3. Heat Exchangers
4. Introduction to Unit Operations
5. *Staged* Unit Operations (distillation, absorption)

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Where do we get the vapor pressure, $p_A^*(T)$?

Raoult's Law

Reference: Felder and Rousseau, 3rd Edition, Section 6.3, Gas-Liquid Systems, One Condensable Component

"A law that describes the behavior of gas-liquid systems over a wide range of conditions provides the desired relationship [between T, P, and y_A]. If a gas at temperature T and pressure P contains a saturated vapor whose mole fraction is y_A (mole vapor/mol total gas), and if this vapor is the only species that would condense if the temperature were slightly lowered, then the partial pressure of the vapor in the gas equals the pure-component vapor pressure $p_A^*(T)$ at the system temperature, [which we look up from tables or data correlations].

Raoult's Law (single condensable component)

$$p_A = y_A P = p_A^*(T)$$

1. Tables (water, Felder and Rousseau, Table B.3)
2. Clausius-Clapeyron equation (constant $\Delta\hat{H}_v$, FR Table B.1)

$$\ln(p^*) = -\frac{\Delta\hat{H}_v}{RT} + B$$

3. Antoine equation (FR Table B.4)

$$\log_{10}(p^*) = A - \frac{B}{T+C}$$

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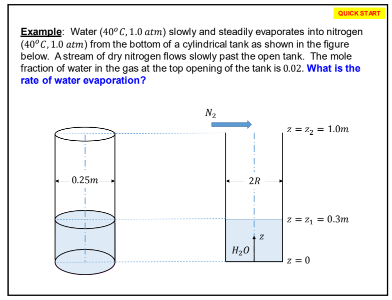
1D Evaporation from tank

Solution:



$$\left(\frac{1-x_A}{1-x_{A1}}\right) = \left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\frac{z-z_1}{z_2-z_1}}$$

Or:

$$x_A = 1-(1-x_{A1})\left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\frac{z-z_1}{z_2-z_1}}$$

Flux of water:

$$N_{Az} = c_1 = \frac{c\mathcal{D}_{AB}}{z_2-z_1}\ln\left(\frac{1-x_{A2}}{1-x_{A1}}\right)$$
$$= 8.0\times 10^{-5}\ mol/m^2 s$$

Rate of evaporation:

$$A_{xs}N_{Az} = 3.9\times 10^{-6} mol/s$$

Note:

$$c = \frac{n}{V} = \frac{P}{RT}$$

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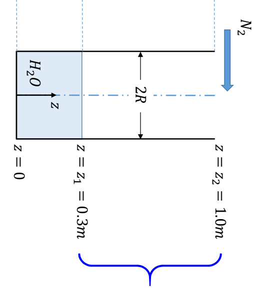
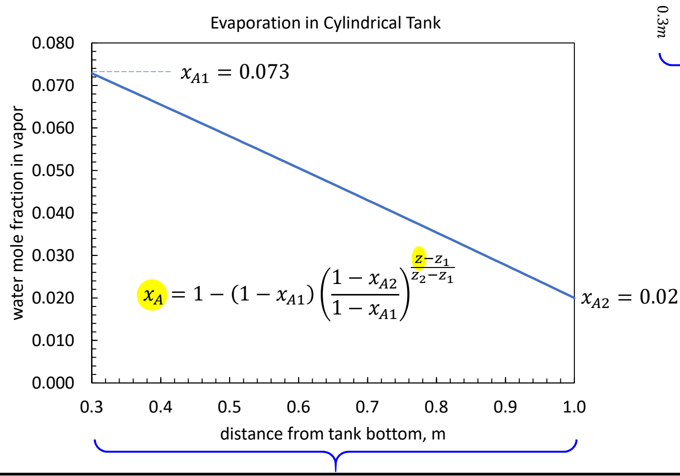
1D Evaporation from tank

What does the solution look like?

$x_{A1} = 0.073$
$x_{A2} = 0.02$
$z_1 = 0.3m$
$z_2 = 1.0m$



Dilute regime:



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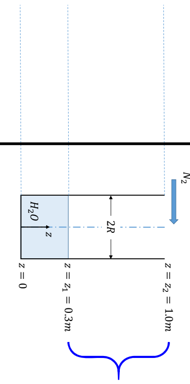
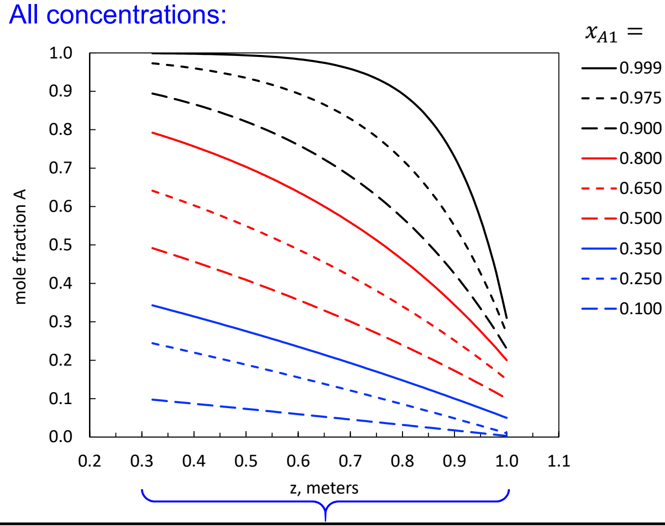
1D Evaporation from tank

What does the solution look like?

$$x_A = 1 - (1 - x_{A1})\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{\frac{z - z_1}{z_2 - z_1}}$$



All concentrations:



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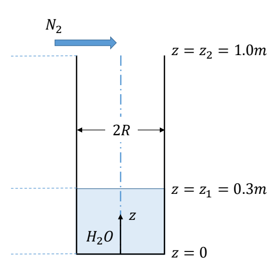
1D Evaporation from tank

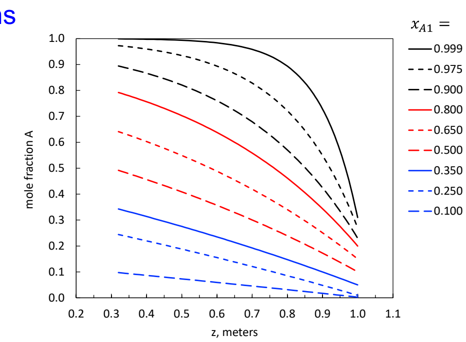
Summary

1D Evaporation from tank



Model:
- 1D diffusion through stagnant layer of B $(N_{Bz} = 0)$
- Steady, no reaction
- Concentration boundary conditions
- Constant $\mathcal{D}_{AB}, c$

Results:
- Constant flux N_{Az}
- Profile depends strongly on BC
- *Linear* profile (like1D rectangular heat transfer) for dilute systems
- *Nonlinear* profile for non-dilute systems



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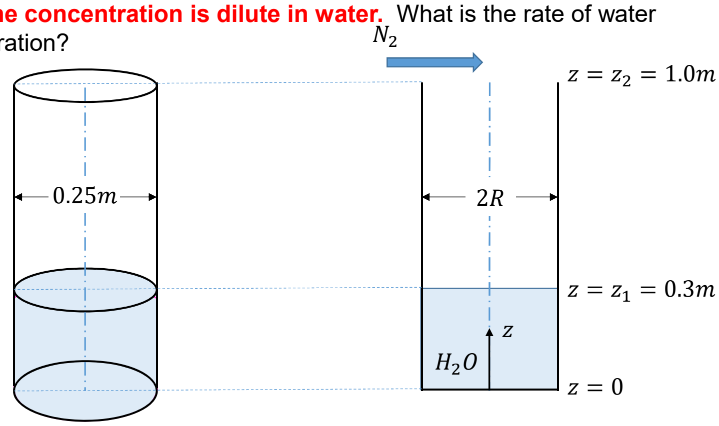
1D Evaporation from tank

QUICK START

Example 1 Redo: Water $(40^oC, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^oC, 1.0\ atm)$ from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. What is water mole fraction as a function of vertical position in the tank? You may assume ideal gas properties **and that the concentration is dilute in water.** What is the rate of water evaporation?



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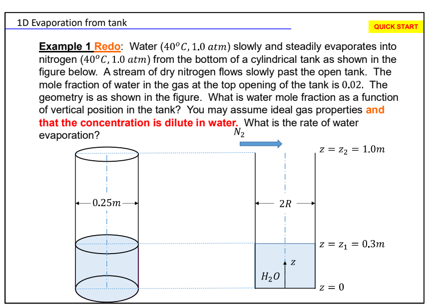
1D Evaporation from tank



Solve.

Answer:

$$\frac{x_A - x_{A1}}{x_{A1} - x_{A2}} = \frac{z - z_1}{z_1 - z_2}$$

or

$$x_A = x_{A1} + (x_{A1} - x_{A2})\left(\frac{z - z_1}{z_1 - z_2}\right)$$

linear

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Next:

1D radial diffusion