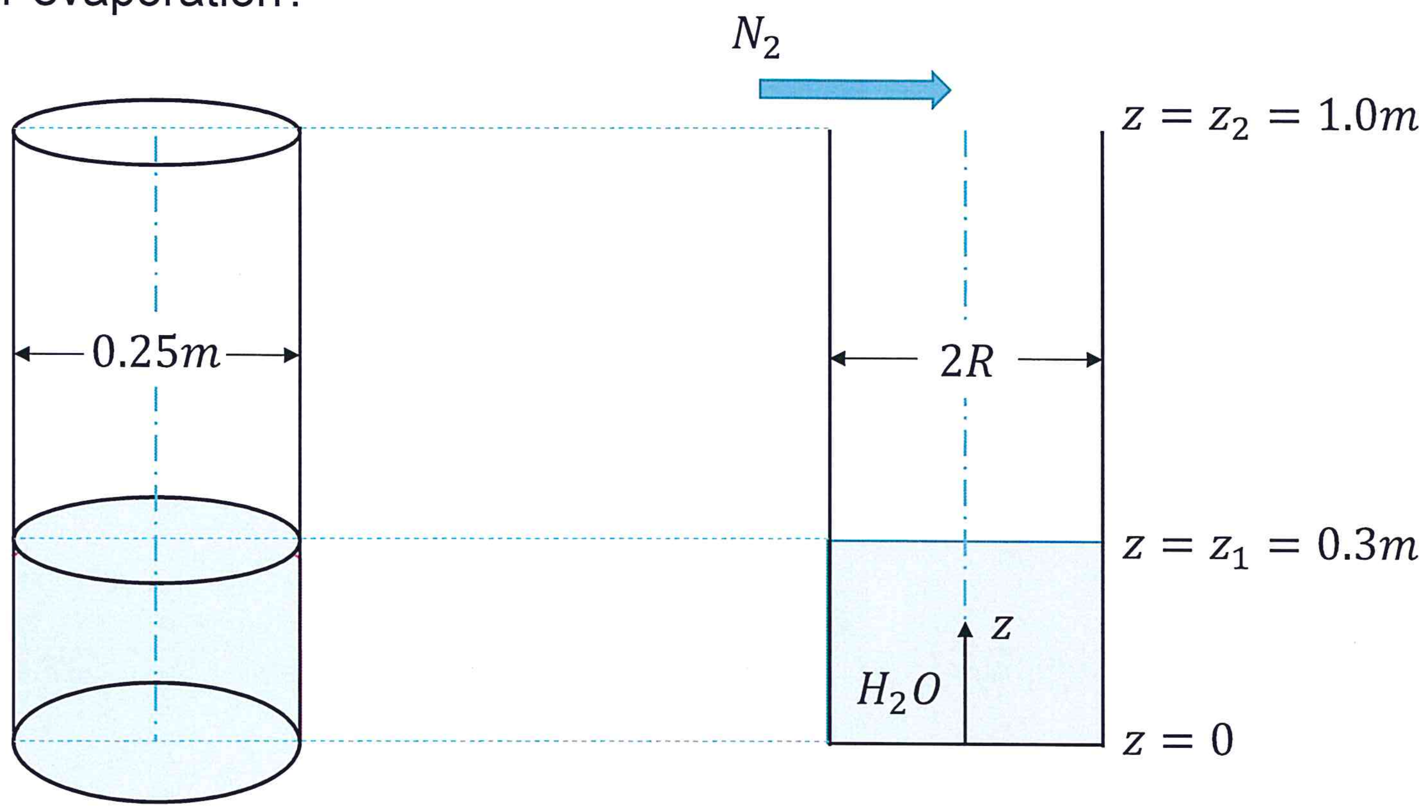
1 MAR 2019 0

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. The geometry is as shown in the figure. What is water mole fraction as a function of vertical position? You may assume ideal gas properties. What is the rate of water evaporation?



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EXAMPLE 1: STEADY DIFFUSION From a Cylindrical Tank

MICRO species "A" mass bal (cylindrical)

see p3

$$\frac{dN_{Az}}{dz} = 0$$

N_{Az} = combined molar flux in z-direction

integrate:

$$\boxed{N_{Az} = c_1}$$

Fick's Law: (cylindrical)

see p3

$$N_{Az} = x_A N_{Az} - cD_{AB} \frac{dx_A}{dz}$$

$$N_{Az} - x_A N_{Az} = -cD_{AB} \frac{dx_A}{dz}$$

③

$$N_{Az}(1-x_A) = -cD_{AB}\frac{dx_A}{dz}$$

from species mass bal → $c_1 = N_{Az}$

$$N_{Az}\,dz = -cD_{AB}\frac{dx_A}{(1-x_A)}$$

$$\int c_1\,dz = -cD_{AB}(-1)\int\frac{-dx_A}{\underbrace{(1-x_A)}_{=u}}$$

$du = -dx_A$

$$c_1 z = +cD_{AB}\ln(1-x_A) + c_2$$

BC: $z = z_2 \quad x_A = 0.02 = x_{A2}$

$z = z_1 \quad x_A = x_A^* = x_{A1}$ ← Raoult's Law

(3)

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

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

no rxn

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

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

θ symmetry

no r-dependence

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:

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

stagnant B

Fick's law of diffusion, spherical coordinates:

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

To Solve:

- substitute
- obtain 2 equations, 2 unknowns
- solve for C_1, C_2

results:
$$\begin{cases} C_1 = \dfrac{c D_{AB}}{(z_1 - z_2)} \ln\left(\dfrac{1 - x_{A1}}{1 - x_{A2}}\right) \\[2ex] C_2 = \ln(1 - x_{A1}) - \dfrac{z_1}{(z_1 - z_2)} \ln\left(\dfrac{1 - x_{A1}}{1 - x_{A2}}\right) \end{cases}$$

- substitute back. Final answer:

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

What is the rate of Evaporation?

Answer: N_{Az}

$\Rightarrow C_1$

$x_{A1} = \frac{P^*}{P} = 0.0728744$ (see tables for $P^*(H_2O, T)$)

$x_{A2} = 0.02$ (given)

$c = \frac{n}{V} = \frac{P}{RT} = 3.891367 \times 10^{-5} \frac{mol}{cm3}$

$P D_{AB} = 2.634 \; m^2 \frac{Pa}{s}$ (App J)

... ANSWER: $\boxed{N_{Az} = 0.026 \; mol/s}$ //