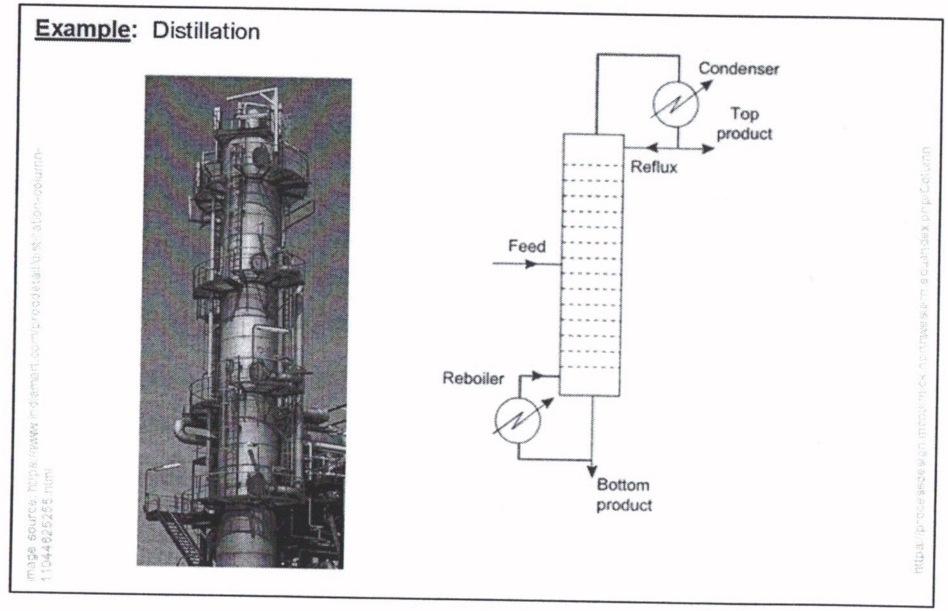
22 MAR 2021 F. MORRISON CM3120 1

Example 4: Mass transfer in distillation

Equimolar Counter Diffusion



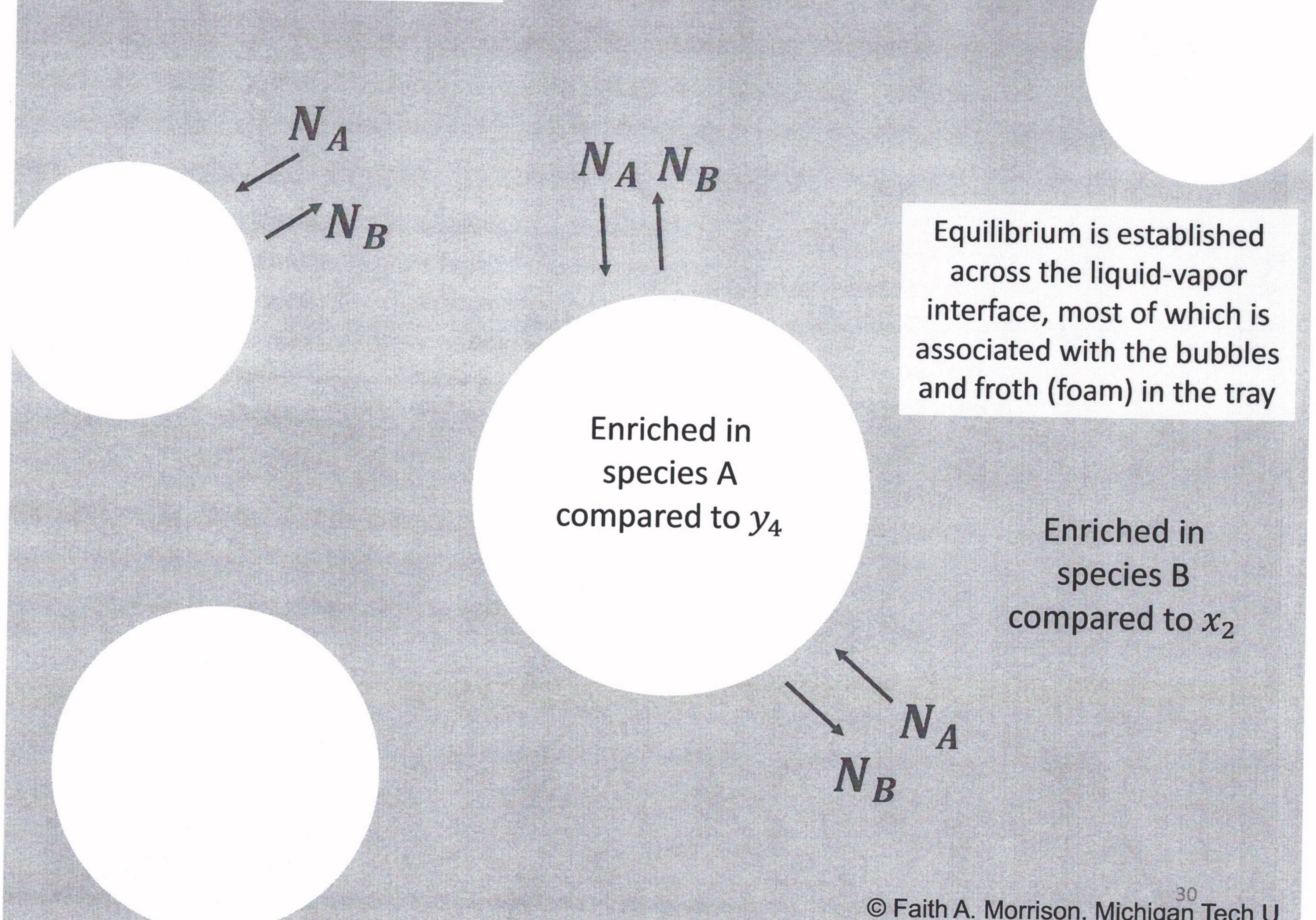
A distillation column is separating two components A and B at steady state. In the vapor phase of each equilibrium stage the two components are moving in **equimolar counter diffusion**. What are the molar fluxes of A and B in the vapor phase? What is the concentration distribution in the region of the equimolar counter diffusion?

⭐ ⇒ MICROSCOPIC SPECIES A MASS BAL!

Wankat, pp110-1

1.1

Equilibrium Stage



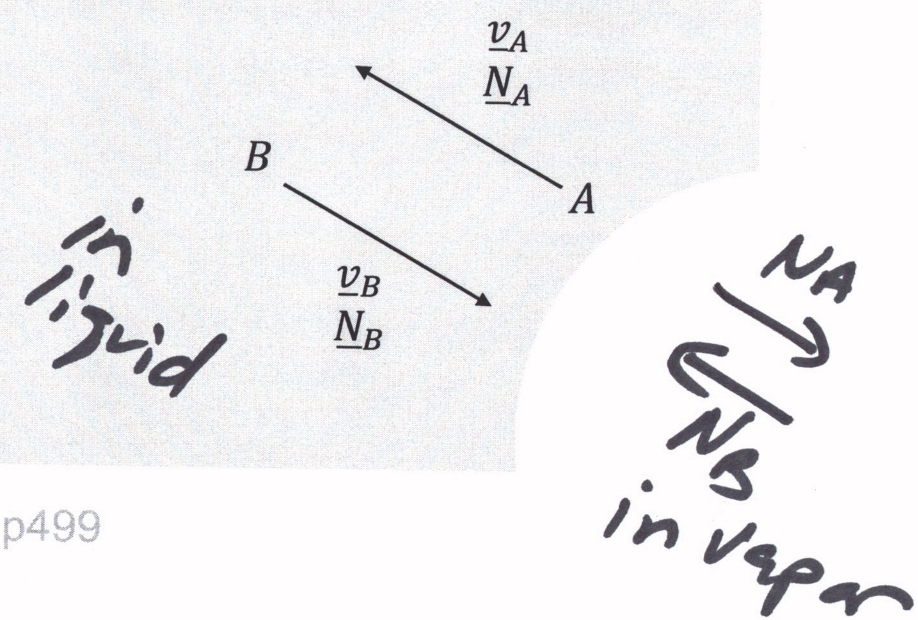
1.2

A Picture of Mass Transfer in Distillation

The molar flow rates throughout the enriching (L, V) and stripping $(\bar{L}, \bar{V})$ sections are constant if:

Every time a mole of vapor is condensed, a mole of liquid is vaporized (**Constant Molal Overflow**)

This condition is met by **equimolar counter diffusion (EMCD)**.



$$\underline{v}_A = -\underline{v}_B$$

$$\underline{N}_A = -\underline{N}_B$$

Note:

$$\underline{N}_A + \underline{N}_B = c\underline{v}^*$$
$$\Rightarrow \underline{v}^* = 0$$

WRF, p499

Equimolar counter diffusion

EMCD:

$$\underline{N}_A = -\underline{N}_B$$

$$\underline{N}_A + \underline{N}_B = 0$$

$$\xrightarrow{N_A}$$

$$\xleftarrow[N_B]{}$$

What is $\underline{N}_A$?

What is x_A?

$z = z_1 \quad x_A = x_{A1}$

$z = z_2 \quad x_A = x_{A2}$

$$\underline{N}_A = \begin{pmatrix} N_{Ax} \\ N_{Ay} \\ N_{Az} \end{pmatrix}_{xyz} = \begin{pmatrix} 0 \\ 0 \\ N_{Az} \end{pmatrix}_{xyz}$$

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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.

Spring 2019 Faith A. Morrison, Michigan Technological University

STEP 1

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

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

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

WRF 25-11

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

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

steady

1D diffusion

no homogeneous rxn

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

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

STEP 2

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

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

WRF 24-22

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ \underbrace{x_A(N_{A,z} + N_{B,z})}_{=0} - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

EMCD

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:

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

MICRO SPECIES A MASS BAL:

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

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

Fick's LAW of Diffusion

$$c_1 = N_{Az} = -c\,D_{AB}\frac{dx_A}{dz}$$

(from sheet)

constant

?

constant

Is c constant?

GAS PHASE (assume ideal)

$$PV = nRT$$

$$c = \frac{P}{RT} = \frac{n}{V} = \frac{\text{moles mix}}{\text{Volume mix}}$$

$\Rightarrow$ constant!

Integrate:

$$\left(-\frac{c_1}{c D_{AB}}\right) = \frac{dx_A}{dz}$$

SOLVE, Apply BC

calc c_1, c_2

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Answers:

$$N_{Az} = \frac{P_{A1} - P_{A2}}{(z_2 - z_1)}\left(\frac{\mathcal{D}_{AB}}{RT}\right)$$

(constant flux proportional to $\mathcal{D}_{AB}$)

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

(linear concentration profile)

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

Wankat, pp110-1