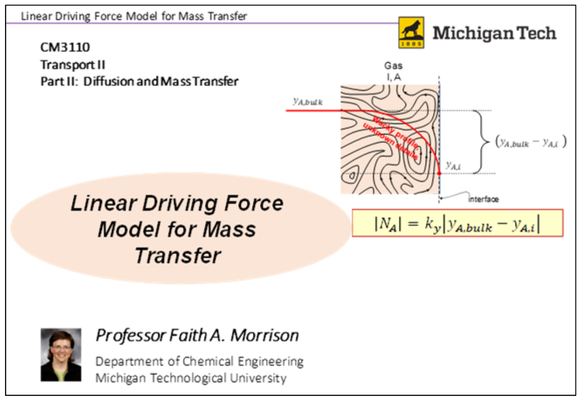
Contining work with the linear driving force for mass transfer, i.e. mass transfer coefficients, k_c



1

Mass Transport "Laws"

Summary

We have 2 Mass Transport "laws"

Transport coefficient

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

Use: Combine with microscopic species A mass balance
Predicts flux $\underline{N}_A$ <u>and</u> composition distributions, e.g. $x_A(x,y,z,t)$
1D Steady models can be solved
1D Unsteady models can be solved (if good at math)
2D steady and unsteady models can be solved by Comsol
Since we predict $\underline{N}_A$, we can also predict a mass xfer coeff k_y or k_c
Diffusion coefficients are ***material*** properties (see tables)

Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

Use: Combine with macroscopic species A mass balance
Predicts flux $\underline{N}_A$, but <u>not</u> composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are ***<u>not</u> material properties***
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G

2

Mass Transport "Laws"

We have 2 Mass Transport "laws"

Transport coefficient

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

Use: ✓Combine with microscopic species A mass balance
Predicts flux $\underline{N}_A$ and composition distributions, e.g. $x_A(x, y, z, t)$
✓ 1D Steady models can be solved
✓ 1D Unsteady models can be solved (if good at math) (2) ✓
2D steady and unsteady models can be solved by Comsol
✓Since we predict $\underline{N}_A$, we can also predict a mass xfer coeff k_y or k_c (1) ✓
Diffusion coefficients are ***material*** properties (see tables)

Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

Use: Combine with macroscopic species A mass balance (3)
Predicts flux $\underline{N}_A$, but not composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are ***not material properties***
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) (4)
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G (5)

3

Mass Transport "Laws"

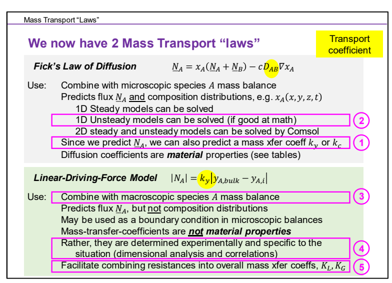
We have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB}

1. ✓ Since we predict $\underline{N}_A$ with Fick's law, we can also predict a mass transfer coefficients k_y or k_c *Relate k_c and D_{AB}*
2. ✓ 1D Unsteady models can be solved (if good at math) *Solutions are analogous to heat transfer*


Mass Transport "Laws"
We now have 2 Mass Transport "laws"
Transport coefficient
Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$
Use: Combine with microscopic species A mass balance
Predicts flux $\underline{N}_A$ and composition distributions, e.g. $x_A(x, y, z, t)$
1D Steady models can be solved
1D Unsteady models can be solved (if good at math) (2)
2D steady and unsteady models can be solved by Comsol
Since we predict $\underline{N}_A$, we can also predict a mass xfer coeff k_y or k_c (1)
Diffusion coefficients are *material* properties (see tables)
Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$
Use: Combine with macroscopic species A mass balance (3)
Predicts flux $\underline{N}_A$, but not composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are *not material properties*
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) (4)
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G (5)

Mass transfer coefficients

k_c

3. Combine with macroscopic species A mass balance
4. Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G, to be used in modeling unit operations

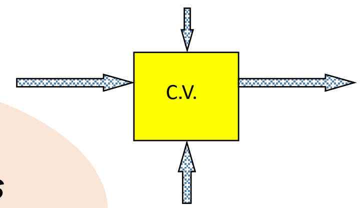
Keep cranking at the list

4

Unsteady Macroscopic Species A Mass Balance

Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer



Macroscopic Species A Mass Balances

3

Professor Faith A. Morrison
Department of Chemical Engineering
Michigan Technological University

5

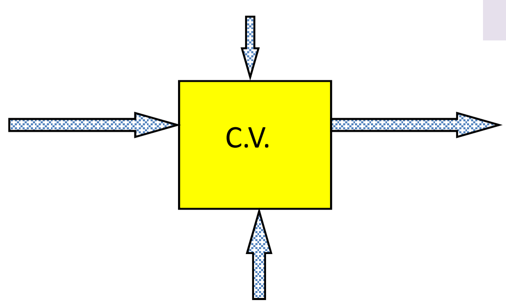
Unsteady Macroscopic Species A Mass Balance

MOLES

**Unsteady,
Macroscopic,
Species A Mass Balance**

balance over
time interval Δt

Macroscopic control volume, C.V.



Keep track of:
- Bulk convection of species A into and out of the C.V.
- Mass transfer across control surfaces of species A
- Mass of species A created by chemical reaction

BSL2, p727
6

Unsteady Macroscopic Species A Mass Balance

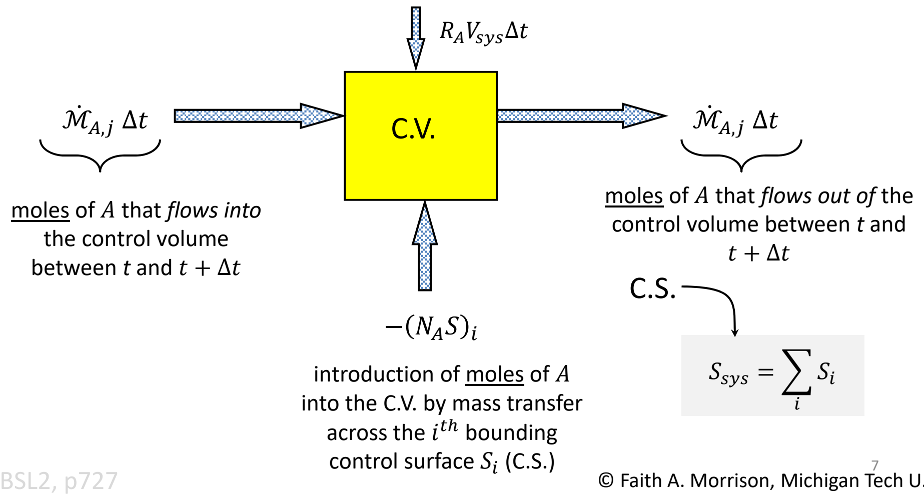
MOLES

Unsteady, Macroscopic, Species A Mass Balance

balance over time interval Δt

Macroscopic control volume, C.V.

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume



BSL2, p727

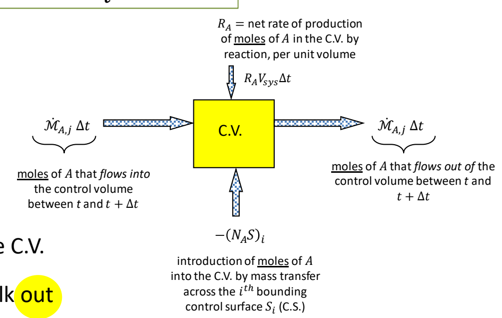
 7

Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_i (N_A S)_i$$



$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs} \dot{\mathcal{M}}_{A,j} - \sum_{j,ins} \dot{\mathcal{M}}_{A,j}$ = bulk out

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

$N_{A_i} = k_c(c_A - c_{Ai}^*)$ =molar flux of A out through the i^{th} C.S.

$S_{sys} = \sum_i S_i$
Δ is "out"- "in"
C.S. = control surface
C.V. = control volume

 8

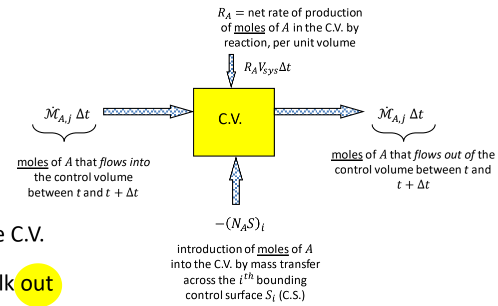
Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_i (N_A S)_i$$

The choice of the "system," i.e. of the *control volume,* is an important first step.



$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs}\dot{\mathcal{M}}_{A,j} - \sum_{j,ins}\dot{\mathcal{M}}_{A,j}$ = bulk out

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

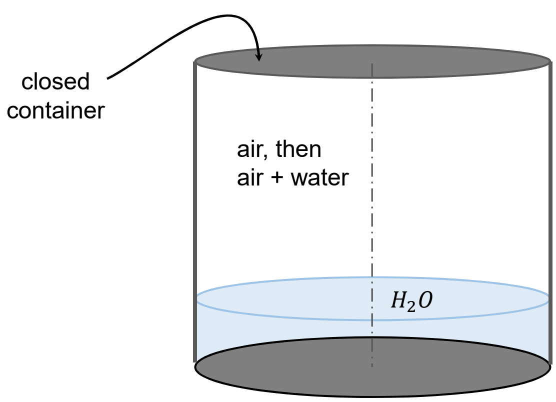
$N_{A_i} = k_c(c_A - c_{Ai}^*)$ =molar flux of A out through the i^{th} C.S.

(think "source" and "sink")

9

Unsteady Macroscopic Species A Mass Balance

Example 8: Bone dry air and liquid water (water volume = $0.80\ liters$) are introduced into a closed container (cross sectional area = $150\ cm^2$; total volume = $19.2\ liters$). Both air and water are at 25^oC, $\sim 1.0\ atm$ throughout this scenario. Three minutes after the air and water are placed in the closed container, the vapor is found to be 5.0% saturated with water vapor. What is the mass transfer coefficient for the water transferring from the liquid to the gas? How long will it take for the gas to become 90% saturated with water?



Cussler, p239, FAM v54 p59

10

Unsteady Macroscopic Species A Mass Balance

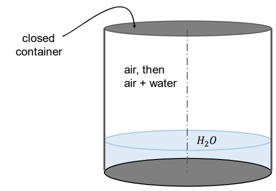
What is our model?

(our assumptions)

1. Control volume =
2.

Unsteady Macroscopic Species A Mass Balance

Example: Bone dry air and liquid water (water volume $= 0.80\ liters$) are introduced into a closed container (cross sectional area $= 150\ cm^2$; total volume $= 19.2\ liters$). Both air and water are at 25^oC throughout this scenario. Three minutes after the air and water are placed in the closed container, the vapor is found to be 5.0% saturated with water vapor. What is the mass transfer coefficient for the water transferring from the liquid to the gas? How long will it take for the gas to become 90% saturated with water?



11

Unsteady Macroscopic Species A Mass Balance

Solution:

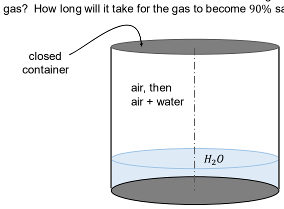
(mass transfer coefficient for evaporating water)

$$\frac{c_A}{c_A^*} = 1 - e^{-\left(\frac{k_c S}{V_{gas}}\right)t}$$

$$t = 2.3\ hours$$

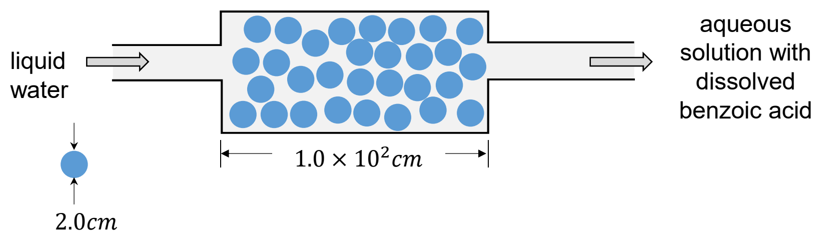
Unsteady Macroscopic Species A Mass Balance

Example: Bone dry air and liquid water (water volume $= 0.80\ liters$) are introduced into a closed container (cross sectional area $= 150\ cm^2$; total volume $= 19.2\ liters$). Both air and water are at 25^oC throughout this scenario. Three minutes after the air and water are placed in the closed container, the vapor is found to be 5.0% saturated with water vapor. What is the mass transfer coefficient for the water transferring from the liquid to the gas? How long will it take for the gas to become 90% saturated with water?



12

Example 9: Flow through a packed bed of soluble spherical pellets.



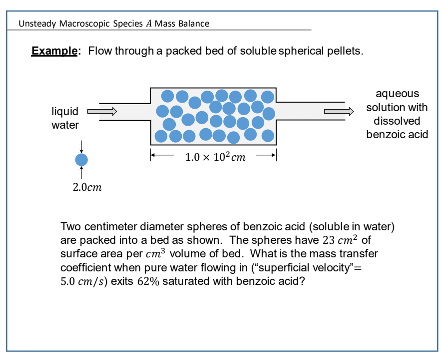
Two-centimeter diameter spheres of benzoic acid (soluble in water) are packed into a bed as shown. The spheres have $23\ cm^2$ of surface area per cm^3 volume of bed. What is the mass transfer coefficient when pure water flowing in ("superficial velocity"= $5.0\ cm/s$) exits 62% saturated with benzoic acid?

Cussler, p240, FAM v54 p63

What is our model?

(our assumptions)

1. Control volume =
2.



Solution:

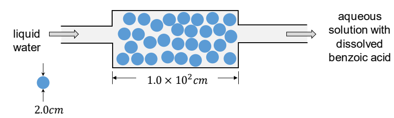
(dissolving benzoic acid in packed bed, pseudo steady state)

$$k_c = \frac{v^0}{aL}\left(-\ln\left(1 - \frac{c_{AL}}{c_A^*}\right)\right)$$

$$k_c = 2.1 \times 10^{-3} cm/s$$

Unsteady Macroscopic Species A Mass Balance

Example: Flow through a packed bed of soluble spherical pellets.



Two centimeter diameter spheres of benzoic acid (soluble in water) are packed into a bed as shown. The spheres have $23\ cm^2$ of surface area per cm^3 volume of bed. What is the mass transfer coefficient when pure water flowing in ("superficial velocity"= $5.0\ cm/s$) exits 62% saturated with benzoic acid?

Example 10: Height of a packed bed absorber

How can we use the linear driving force model for mass transfer to design a packed bed gas absorber to achieve a desired separation?

BSL2 p742

Unsteady Macroscopic Species A Mass Balance

Example 10: Height of a packed bed absorber

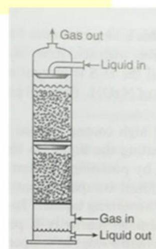
How can we use the linear driving force model for mass transfer to design a packed bed gas absorber to achieve a desired separation?

From lecture 8:

Gas Absorption

While a chemical plant would not exist without the chemical reactors, the biggest expense (the biggest equipment) will often be the separation equipment, **distillation columns** and **gas absorption columns**.

- Packed column (tower)
- Liquid poured into top trickles down through packing
- Gas pumped into bottom flows upward
- Analysis involves both **fluid mechanics** (determines cross-sectional area) and **mass transfer** (determines height)



BSL2 p742

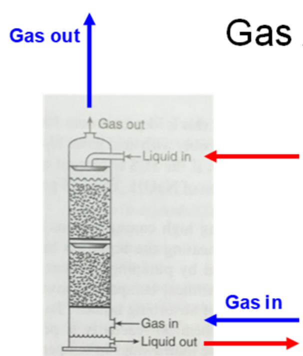
17

Unsteady Macroscopic Species A Mass Balance—Gas Absorption

From lecture 8:

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Gas Absorption



Exiting liquid stream contains high concentrations of the impurity.

Cussler, p307

18

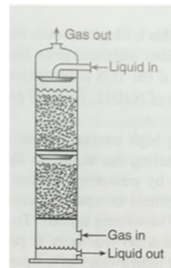
Unsteady Macroscopic Species A Mass Balance—Gas Absorption

From lecture 8:

Gas Absorption

Gas Absorption Tower Design

A type of “differential contacting”



Design: Diameter, Height

Complicated; solved by trial and error

- Diameter: constrained by the fluid mechanics of the gas and liquid flowing past each other; complicated; described by largely empirical correlations (use turnkey procedure)
- Height: must be sufficient to attain the separation desired; depends on how solubility depends on concentration (linear or nonlinear isotherm, dilute (easy), not dilute (hard))

Can be modeled.

Cussler, p304

19

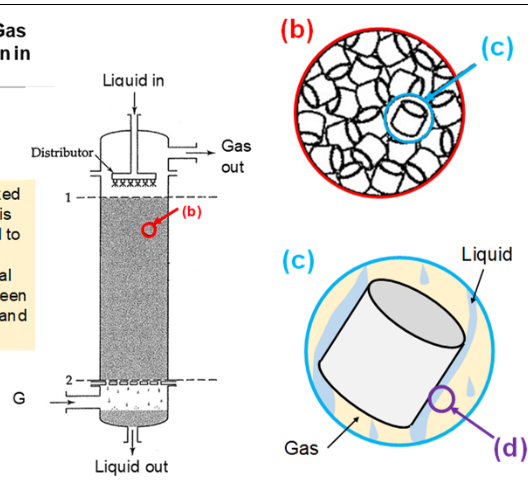
Unsteady Macroscopic Species A Mass Balance—Gas Absorption

From lecture 8:

Model of Gas Absorption in a Column

(a) Column

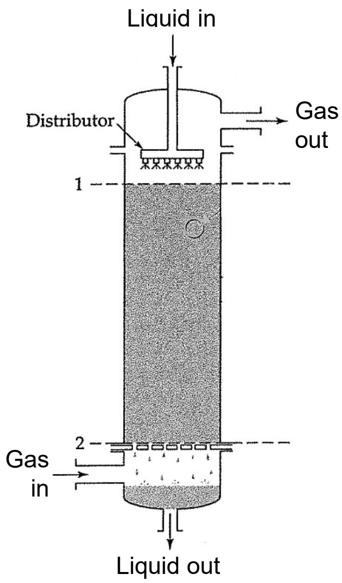
The packed column is designed to create interfacial area between the liquid and gas.



BSL2, p743

20

Unsteady Macroscopic Species A Mass Balance—Gas Absorption

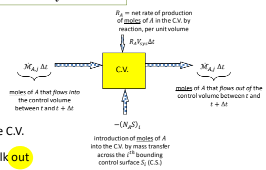


Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_i (N_A S)_i$$



$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs}\dot{\mathcal{M}}_{A,j} - \sum_{j,ins}\dot{\mathcal{M}}_{A,j}$ = bulk out

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

$N_{A_i} = k_c(c_A - c_{Ai}^*)$ =molar flux of A out through the i^{th} C.S.

$S_{sys} = \sum_i S_i$
Δ is "out"- "in"
C.S. = control surface
C.V. = control volume

?

You try.

21

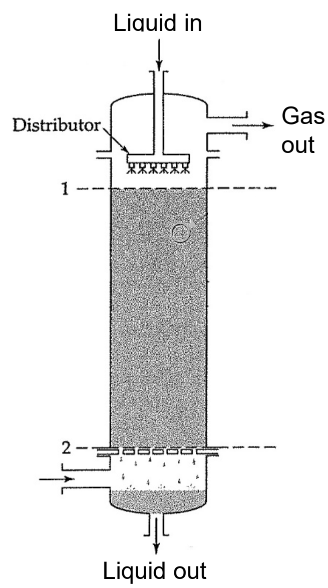
© Faith A. Morrison, Michigan Tech U.

Unsteady Macroscopic Species A Mass Balance

What is our model?

(our assumptions)

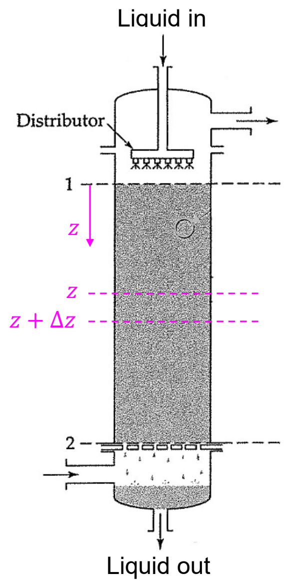
1. Control volume =
2.



22

© Faith A. Morrison, Michigan Tech U.

Unsteady Macroscopic Species A Mass Balance—Gas Absorption



Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_i (N_A S)_i$$

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

$R_A V_{sys} \Delta t$

$\dot{\mathcal{M}}_{A,j}\,\Delta t$ — moles of A that *flows into* the control volume between t and $t + \Delta t$

C.V.

$\dot{\mathcal{M}}_{A,j}\,\Delta t$ — moles of A that *flows out of* the control volume between t and $t + \Delta t$

$-(N_A S)_i$ — introduction of moles of A into the C.V. by mass transfer across the i^{th} bounding control surface S_i (C.S.)

$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

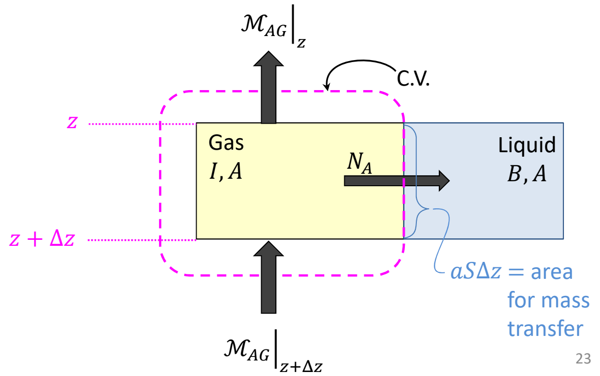
$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs}\dot{\mathcal{M}}_{A,j} - \sum_{j,ins}\dot{\mathcal{M}}_{A,j}$ = bulk out

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

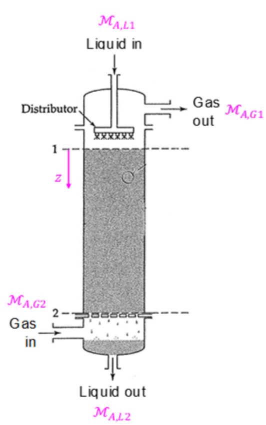
$N_{A_i} = k_c(c_A - c_{Ai}^*)$ =molar flux of A out through the i^{th} C.S.

$S_{sys} = \sum_i S_i$
Δ is "out"- "in"
C.S. = control surface
C.V. = control volume



23

Unsteady Macroscopic Species A Mass Balance—Gas Absorption



$\mathcal{M}_G \equiv$ moles gas on an A-free basis

$$\mathcal{Y}_A \equiv \frac{y_A}{y_I} = \frac{y_A}{1-y_A}$$

$$\mathcal{X}_A \equiv \frac{x_A}{x_B} = \frac{x_A}{1-x_A}$$

} molar ratios

$\mathcal{Y}_A \approx y_A$ for dilute systems

$$\mathcal{X}_A = \mathcal{X}_{A1} + \frac{\mathcal{M}_G}{\mathcal{M}_L}\left(\mathcal{Y}_A - \mathcal{Y}_{A1}\right)$$

(Operating line; from mass balance on the top of the column)

$$\frac{k_x a}{k_y a} = \frac{\mathcal{Y}_A - \mathcal{Y}_A^*}{\mathcal{X}_A - \mathcal{X}_A^*}$$

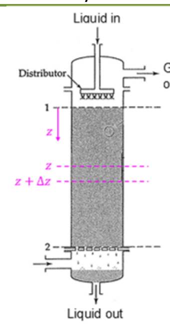
(result from $N_{A,gas} = -N_{A,liquid}$; BSL's equation 23.5-21)

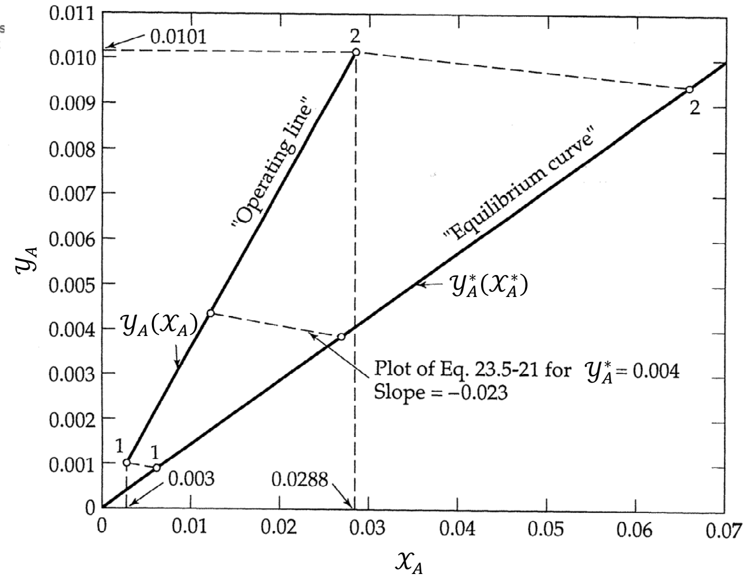
…

BSL2 p745

24

Unsteady Macroscopic Species A Mass Balance—Gas Absorption





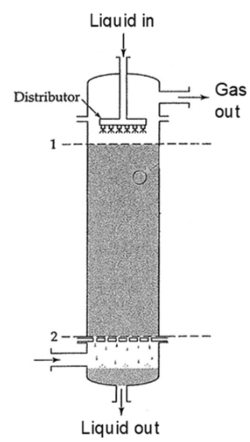
BSL2 p745 Bird, Stewart, and Lightfoot, Transport Phenomena, 2nd ed., Wiley, 2006.

25

Unsteady Macroscopic Species A Mass Balance

Solution:

(height of a packed bed absorber)



Answer: Perform numerical integration to obtain the column height L:

$$L = \frac{\mathcal{M}_G}{(k_y a)S} \int_{\mathcal{Y}_{A1}}^{\mathcal{Y}_{A2}} \frac{d\mathcal{Y}_A}{(\mathcal{Y}_A - \mathcal{Y}_A^*)}$$

Need: Gas flow rate $\mathcal{M}_G$, column cross sectional area S, data on thermodynamic equilibrium $\mathcal{Y}_A^*(\mathcal{X}_A^*)$, desired separation (mole fractions top and bottom, and mass transfer coefficients $k_y a$ and $k_x a$.

26

Mass Transport "Laws"

We have 2 Mass Transport "laws"

Transport coefficient

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

Use: ✓Combine with microscopic species A mass balance
Predicts flux $\underline{N}_A$ and composition distributions, e.g. $x_A(x, y, z, t)$
✓ 1D Steady models can be solved
✓ 1D Unsteady models can be solved (if good at math) (2) ✓
2D steady and unsteady models can be solved by Comsol
✓Since we predict $\underline{N}_A$, we can also predict a mass xfer coeff k_y or k_c (1) ✓
Diffusion coefficients are ***material*** properties (see tables)

Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

Use: ✓Combine with macroscopic species A mass balance (3) ✓
Predicts flux $\underline{N}_A$, but not composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are ***not material properties***
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) (4)
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G (5)

27

Mass Transport "Laws"

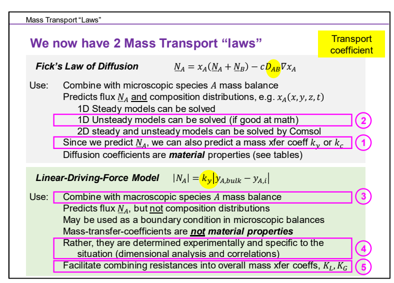
We have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB}

1. ✓Since we predict $\underline{N}_A$ with Fick's law, we can also predict a mass transfer coefficients k_y or k_c *Relate k_c and D_{AB}*
2. ✓1D Unsteady models can be solved (if good at math) *Solutions are analogous to heat transfer*


Mass Transport "Laws"
We now have 2 Mass Transport "laws"
Transport coefficient
Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$
Use: Combine with microscopic species A mass balance
Predicts flux $\underline{N}_A$ and composition distributions, e.g. $x_A(x, y, z, t)$
1D Steady models can be solved
1D Unsteady models can be solved (if good at math) (2)
2D steady and unsteady models can be solved by Comsol
Since we predict $\underline{N}_A$, we can also predict a mass xfer coeff k_y or k_c (1)
Diffusion coefficients are *material* properties (see tables)
Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$
Use: Combine with macroscopic species A mass balance (3)
Predicts flux $\underline{N}_A$, but not composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are ***not material properties***
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) (4)
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G (5)

Mass transfer coefficients

k_c

3. ✓Combine with macroscopic species A mass balance *Model macroscopic processes; design units*
4. Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G, to be used in modeling unit operations

28