CM3120: Module 4

Diffusion and Mass Transfer II

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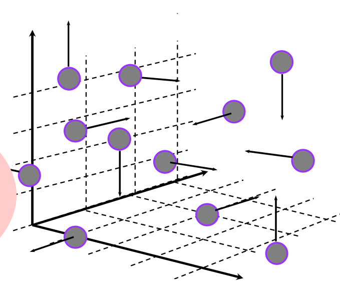
Module 4 Lecture II

Classics Diffusion & Mass Transfer

(Penetration, Gas Absorption)



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Michigan Technological University

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

Classic 1D Steady Diffusion Summary

a. 1D rectangular mass transfer (evaporating tank, **Ex 1**)

b. 1D radial mass transfer (evaporating droplet, **Ex 2**)

c. Heterogeneous chemical reaction (catalytic converter, **Ex 3**)

d. Equimolar counter diffusion (distillation, $\underline{v}^* = 0,\ (\underline{N}_A = \underline{J}_A^*)$ **Ex 4**)

Next:

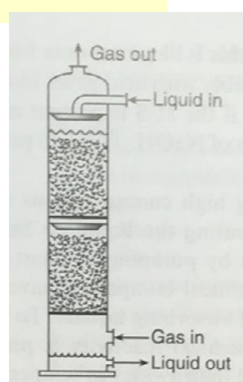
e. Homogeneous chemical reaction, penetration model (gas absorption by chemical solvent, **Ex 5**)

Gas Absorption

Image source: www.sulzer.com

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** (cross-sectional area chosen to avoid flooding) and **mass transfer** (height adjusted to achieve desired separation)

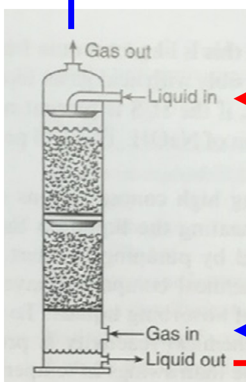


Cussler, p305, 7

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Gas Absorption

Gas out



Liquid in

Gas in

Liquid out

Exiting liquid stream contains high concentrations of the impurity. This is later “stripped” by heating the liquid so that the impurity bubbles out.

The “swing” in temperature may sometimes be replaced by a “swing” in pressure (lowers costs)

Cussler, p307

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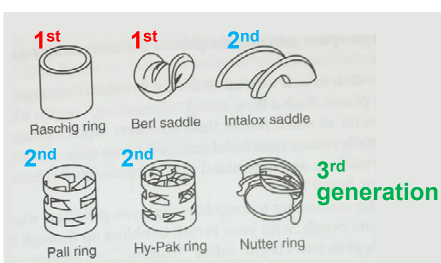
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Designed by 80 years of experience

Gas Absorption Packing

- Packing is designed to create a large amount of gas-liquid contact area
- High fluid flow trades off with high interfacial area (both are desired)
- High fluid flow rates can lead to column flooding



6 types of random packing; cheaper, common

Image source: www.sulzer.com

Structured packing; pricey, more efficient (up to 30% more efficient); fluids move past each other with less bypassing

Cussler, p308,9

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Gas Absorption- the liquids

What are the gases to be absorbed?
*What are the **liquids** that absorb them?*

Some depend on the solubility of the gas
Most react chemically with the components of the gas

Choice depends on the concentrations in the feed gas mixture and on the desired percent removal

High concentration (10-50%): dissolve in a nonvolatile, nonreactive liquid, aka **physical solvent** *(less common, but simpler)*

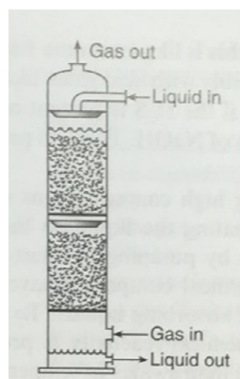
Lower concentration (1-10%): use liquid capable of fast, reversible chemical reaction with the gas to be removed, aka **chemical solvent** *(20X more common, but complex)*

Very low concentration (<1%): use an adsorbent that reacts irreversibly (this is expensive; may produce solid waste).

Cussler, p306,7

Gas Absorption Tower Design

A type of "differential contacting" (not staged)



Design: Diameter, Height

Diameter:
- constrained by the fluid mechanics of the gas and liquid flowing past each other;
- want sufficient contact so that mass transfer takes place;
- flooding to be avoided;
- complicated;
- described by largely empirical correlations (use turnkey procedure)

Height:
- must be sufficient to attain the separation desired given the mass-transfer performance of the packing;
- depends on how solubility depends on concentration (dilute (easy), not dilute (hard))

Cussler, p304

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Gas Absorption Tower Design

A type of "differential contacting" (not staged)

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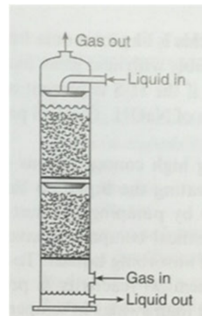
- constrained by the fluid mechanics of the gas and liquid flowing past each other;
- want sufficient contact so that mass transfer takes place;
- flooding to be avoided;
- complicated;
- described by largely empirical correlations (use turnkey procedure)

Complicated; solved by trial and error (by vendors)

Height:
- must be sufficient to attain the separation desired given the mass-transfer performance of the packing;
- depends on how solubility depends on concentration (dilute (easy), not dilute (hard))

Can be modeled.



Cussler, p304

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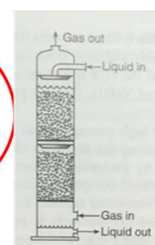
1D Steady Diffusion—Gas Absorption

Column height must be sufficient to attain the separation desired.

Design: Diameter, Height

Height:
- must be sufficient to attain the separation desired given the mass-transfer performance of the packing;
- depends on how solubility depends on concentration (dilute (easy), not dilute (hard))



We need a *model* of how the separation is achieved to produce the design equations for the height of the column.

A model that **works** will reveal what the physics of the unit is.

Models that **only partially work** also reveal important aspects of the physics.

Cussler, p304

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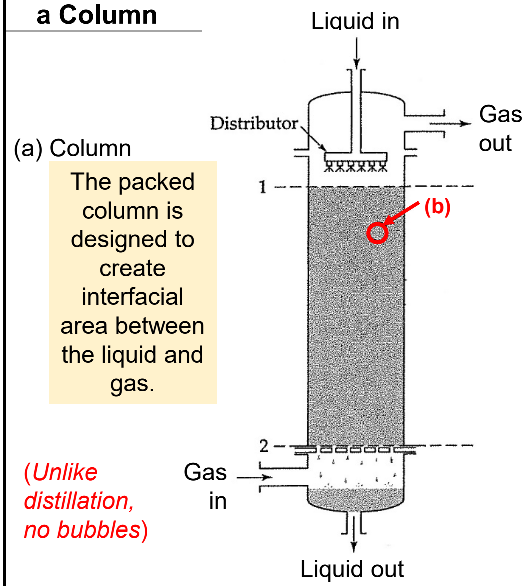
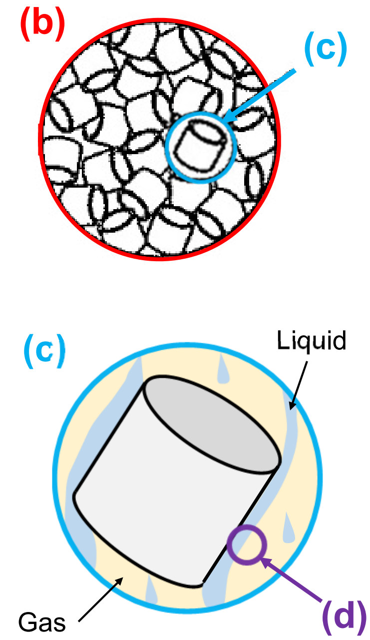
Model of Gas Absorption in a Column





BSL2, p743

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1D Steady Diffusion—Gas Absorption with Chemical Solvent

The Mass-Transfer Model

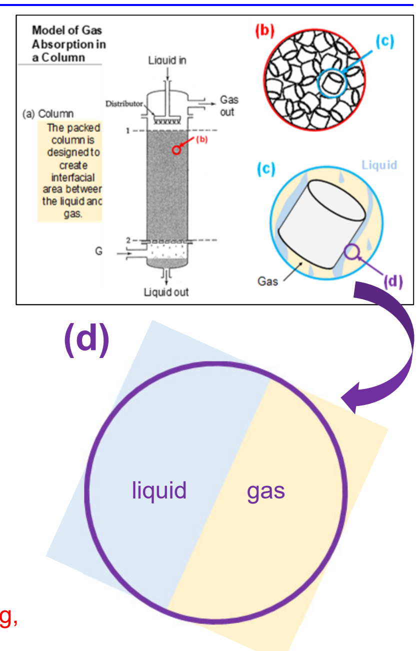
We focus on the **liquid-gas interface** where the mass transfer takes place.

Idealize the **entire device** as comprising only the appropriate amount of this interface, with mass transfer taking place there.

Retain the role of the column, by forcing the appropriate concentrations of species A to enter and exit the column.

$$a \equiv \frac{\text{interfacial area}}{\text{volume}}$$

A property of the column and packing, in operation



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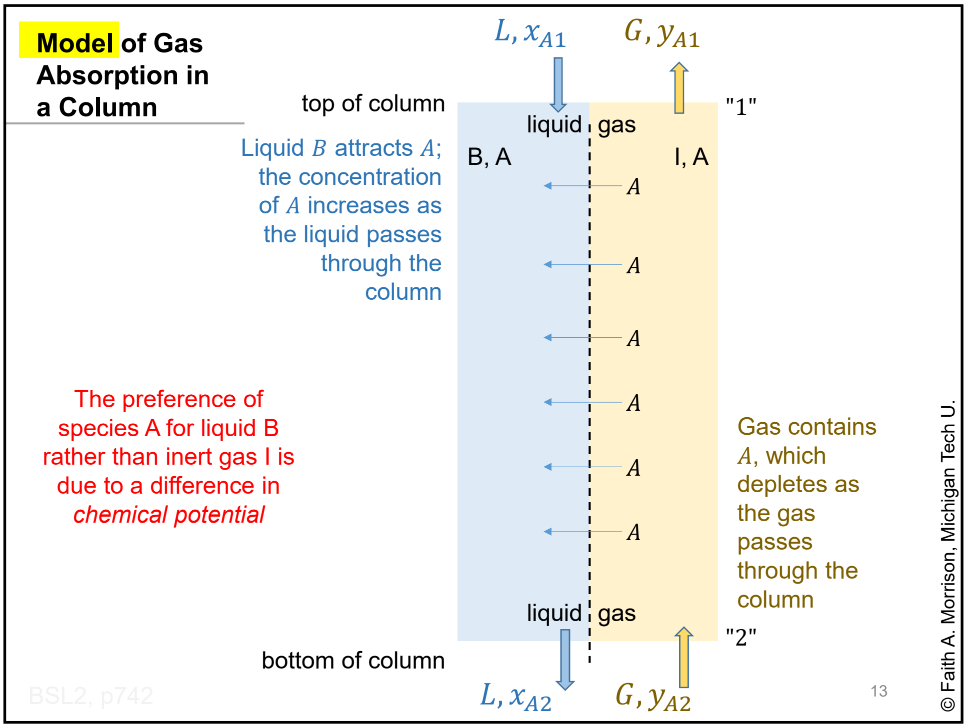
Model of Gas Absorption in a Column
L, x_{A1}
G, y_{A1}
top of column
"1"
liquid
gas
B, A
I, A
Liquid B attracts A; the concentration of A increases as the liquid passes through the column
A
A
A
A
A
A
The preference of species A for liquid B rather than inert gas I is due to a difference in *chemical potential*
Gas contains A, which depletes as the gas passes through the column
liquid
gas
"2"
bottom of column
L, x_{A2}
G, y_{A2}
BSL2, p742
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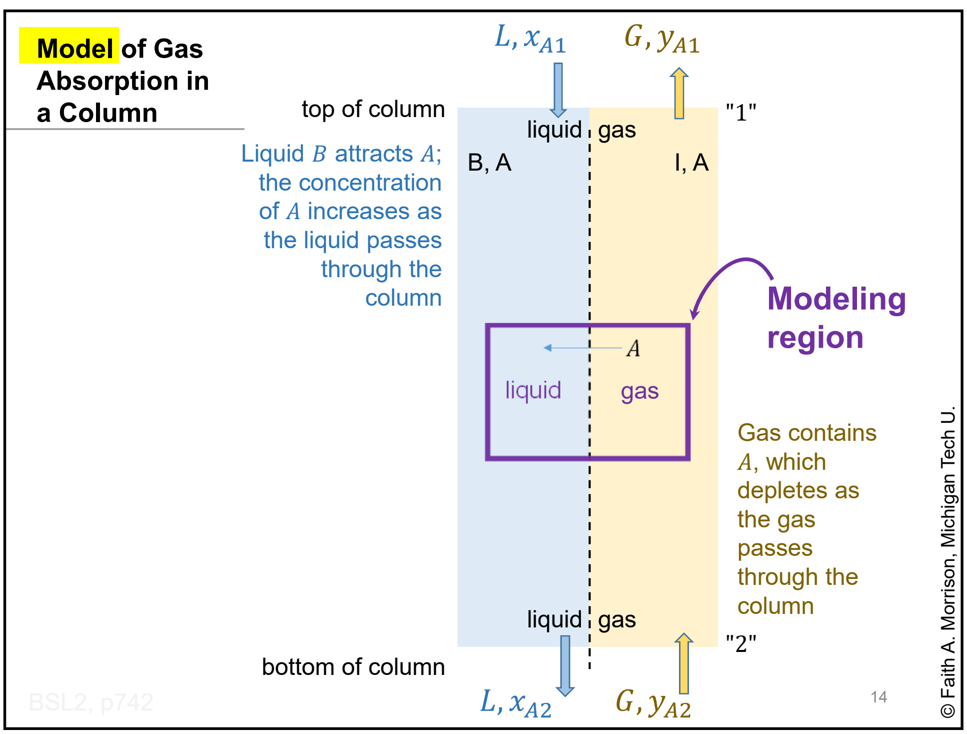
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Modeling region
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Gas contains A, which depletes as the gas passes through the column
liquid
gas
"2"
bottom of column
L, x_{A2}
G, y_{A2}
BSL2, p742
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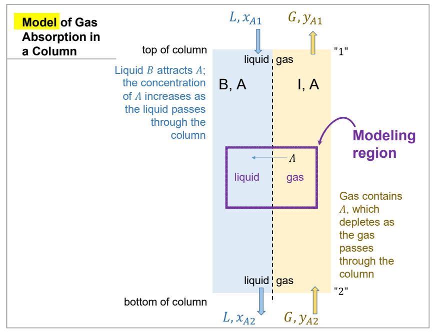
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example 5: Mass transfer a Gas Absorption Column (Chemical Solvent)



A gas absorption column is operating at steady state. The gas stream is composed of component A and an inert carrier gas I. The liquid stream is chemical absorbent B. Component A diffuses across the gas-liquid interface until it reacts with B. What are the molar fluxes of A and B? What is the concentration distribution in the region in which A diffuses into liquid B?

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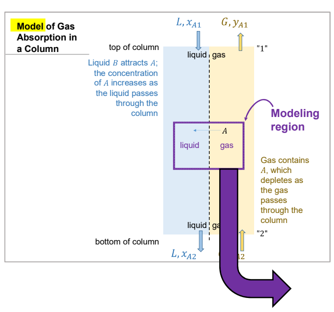
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example 5: Gas Absorption Column



The action of the chemical solvent B (absorbent) modeled as a homogeneous chemical reaction taking place in the penetration region.

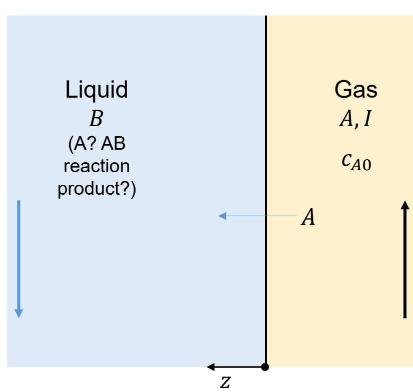
$$A + B \rightarrow AB$$

$$R_A = -k_1 c_A$$

How can we visualize (model) this happening?

What questions can we ask?

(dilute A)



WRF p505

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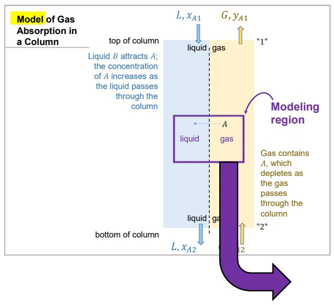
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example 5: Gas Absorption Column

Use a "*penetration model*"



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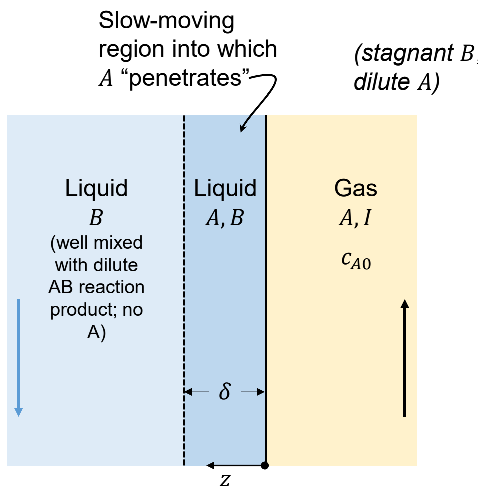

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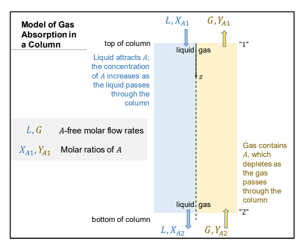
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example 5: Mass transfer a Gas Absorption Column (Chemical Solvent)



A gas absorption column is operating at steady state. The gas stream is composed of component A and an inert carrier gas I. The liquid stream is chemical absorbent B. Component A diffuses across the gas-liquid interface until it reacts with B. What are the molar fluxes of A and B? What is the concentration distribution in the region in which A diffuses into liquid B?

Solve

See hand notes for the start

Homework 4 Problem 4.3

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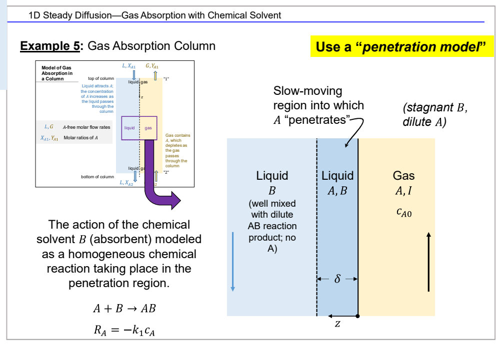
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Problem Summary: Gas Absorption with Chemical Solvent

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux $\underline{N}_A$)
- Needed stoichiometry and rate equation
- Boundary conditions: concentrations known (A disappears at penetration length)

Flux choice
Choose:
- **Molar** because there is a reaction
- **Combined molar** because there is no imposed bulk convection; A is dilute; A moves through stagnant B



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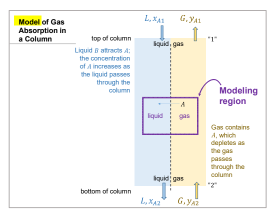
1D Steady Diffusion—Penetration model

Analysis



Assuming penetration model (irreversible chemical reaction) for gas absorption implies hyperbolic sinh, cosh concentration profile.

$$c_A(z) = c_{A0}\cosh\left(z\sqrt{k_1/\mathcal{D}_{AB}}\right) - \frac{c_{A0}\sinh\left(z\sqrt{k_1/\mathcal{D}_{AB}}\right)}{\tanh\left(\delta\sqrt{k_1/\mathcal{D}_{AB}}\right)}$$

WRF p506

And variable flux proportional to the concentration gradient

$$N_{Az} = -\mathcal{D}_{AB}\frac{dc_A}{dz}$$

At the interface ($z = 0$) this becomes

$$N_{A0} = \frac{\mathcal{D}_{AB}c_{A0}\sqrt{k_1/\mathcal{D}_{AB}}}{\tanh\left(\delta\sqrt{k_1/\mathcal{D}_{AB}}\right)}$$

For large k_1, $\tanh\left(\delta\sqrt{k_1/\mathcal{D}_{AB}}\right) \rightarrow 1$, and

$$N_{A0} = c_{A0}(k_1\mathcal{D}_{AB})^{\frac{1}{2}}$$

Again, this modeling effort tells us how a material property, $\mathcal{D}_{AB}$, relates to the concentration distribution and flux for this idealized case. We need to check if true.

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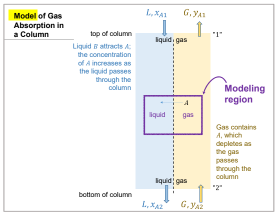
1D Steady Diffusion—Penetration model



Analysis

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Again, this modeling effort tells us how a material property, $\mathcal{D}_{AB}$, relates to the concentration distribution and flux for this idealized case. We need to check if true.

But,

- It's hard to measure the flux inside a gas absorber (packed tower).
- Later we will define some macroscopic mass transfer methods that we can use to asses the degree to which penetration model seems consistent with measurements for gas absorption (mass transfer coefficients and how they depend on D_{AB})
- For now, we can just hold onto penetration model as an idea of how mass transfer works in an absorption column.

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1D Steady Diffusion

Classic 1D Steady Diffusion Summary

a. 1D rectangular mass transfer (evaporating tank, **Ex 1**)

b. 1D radial mass transfer (evaporating droplet, **Ex 2**)

c. Heterogeneous chemical reaction (catalytic converter, **Ex 3**)

d. Equimolar counter diffusion (distillation, $\underline{v}^* = 0$, $(\underline{N}_A = \underline{J}_A^*)$ **Ex 4**)

e. Homogeneous chemical reaction, penetration model (gas absorption by chemical solvent, **Ex 5**)

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Introduction to Diffusion and Mass Transfer in Mixtures

QUICK START

Recurring Modeling Assumptions in Diffusion ("Classics")

- Near a liquid-gas interface, the region in the gas near the liquid is a film where slow diffusion takes place
- The vapor near the liquid-gas interface is often saturated (Raoult's law, $x_A = p_A^*/p$)
- If component A has no sink, flux $\underline{N}_A = 0$
- If A diffuses through stagnant B, $\underline{N}_B = 0$
- If A is dilute in B, we can neglect the convection term, yielding $N_{Az} = J_{Az}^*$; also liquid concentration c will be constant in the dilute case
- Because diffusion is slow, we can make a quasi-steady-state assumption
- 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 $-0.5\underline{N}_A = \underline{N}_B$.
- Homogeneous reactions appear in the mass balance; heterogeneous reactions appear in the boundary conditions and relate fluxes
- If a binary mixture of A and B are undergoing steady equimolar counter diffusion, $\underline{N}_A = -\underline{N}_B$
- Penetration model is a viable perspective for some homogeneous reaction systems (e.g. gas absorption)

DONE (end of classics)//

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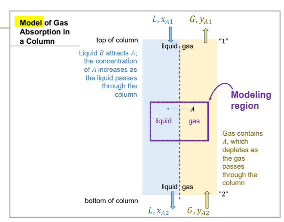
Distillation modeling: EMCD

Gas Absorber Modeling Summary



- Absorber modeling with actual packing dynamics replaced with gas-liquid contacting gives a plausible picture of the unit operation
- Penetration model (irreversible reaction) is the mass transfer picture
- Penetration model is a "classic" of diffusion and mass transfer
- The penetration model is idealized mass transfer; the packing details determine the mass transfer separation efficiency
- Both gas absorption and distillation columns these days are packed columns; we will have to consider a different model for packed columns

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