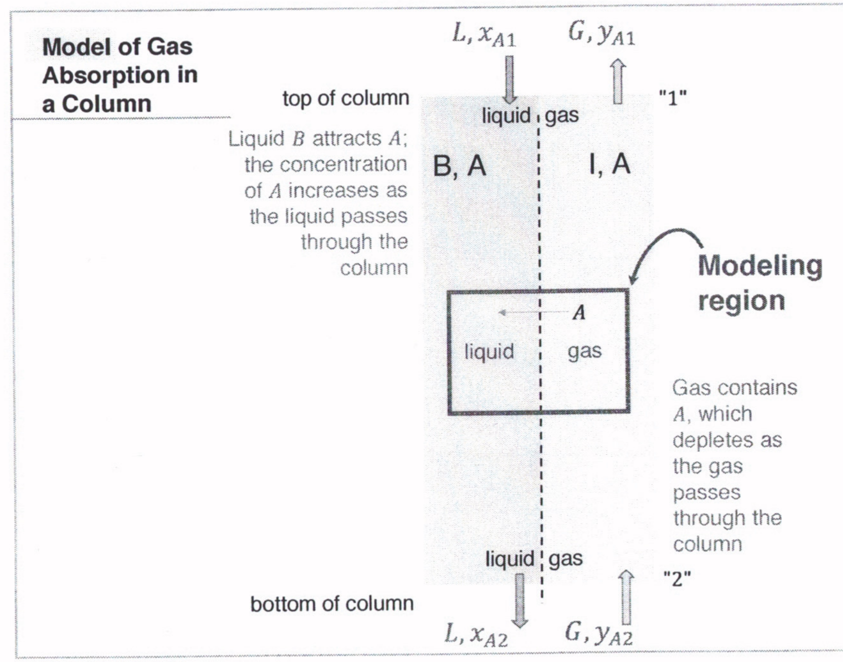
Example 5: Mass transfer a Gas Absorption Column (Chemical Solvent)

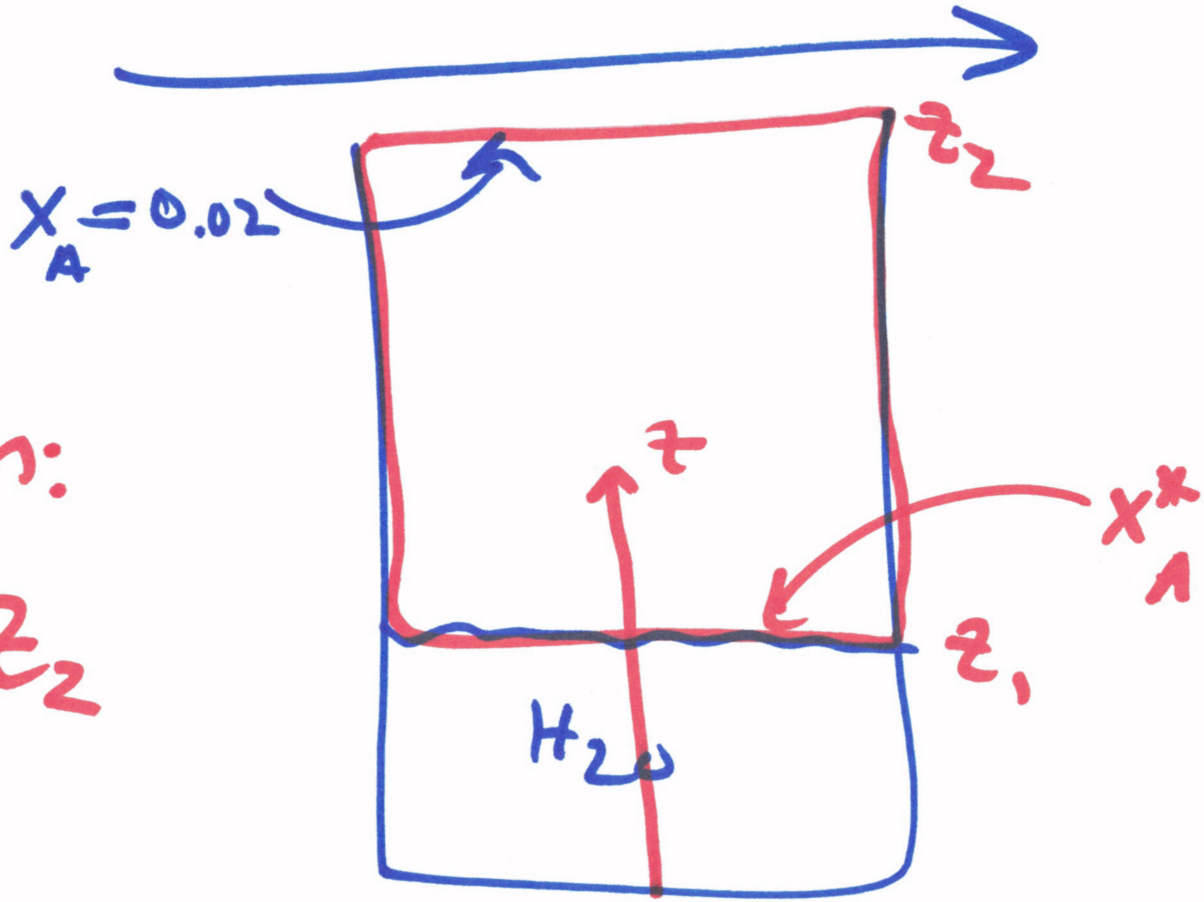


A gas absorption column is operating at steady state. The gas stream is composed of component A and an inert carrier gas I. The liquid stream is chemical absorbent B. Component A diffuses across the gas-liquid interface until it reacts with B. What are the molar fluxes of A and B? What is the concentration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

Wankat, pp110-1

THINK BACK: How to model? Review past models:

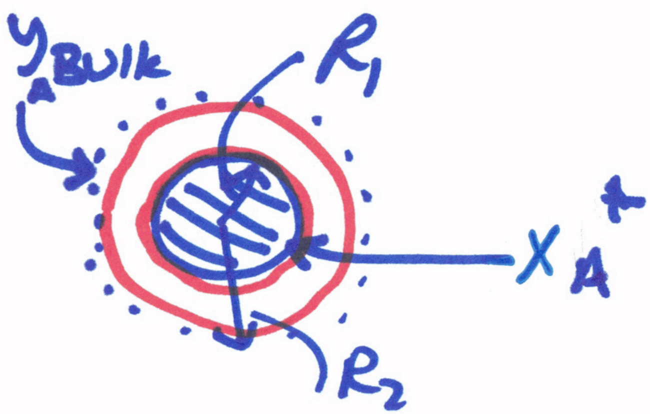
→ Ex 1:



domain:

$z_1 < z < z_2$

→ Ex 2:

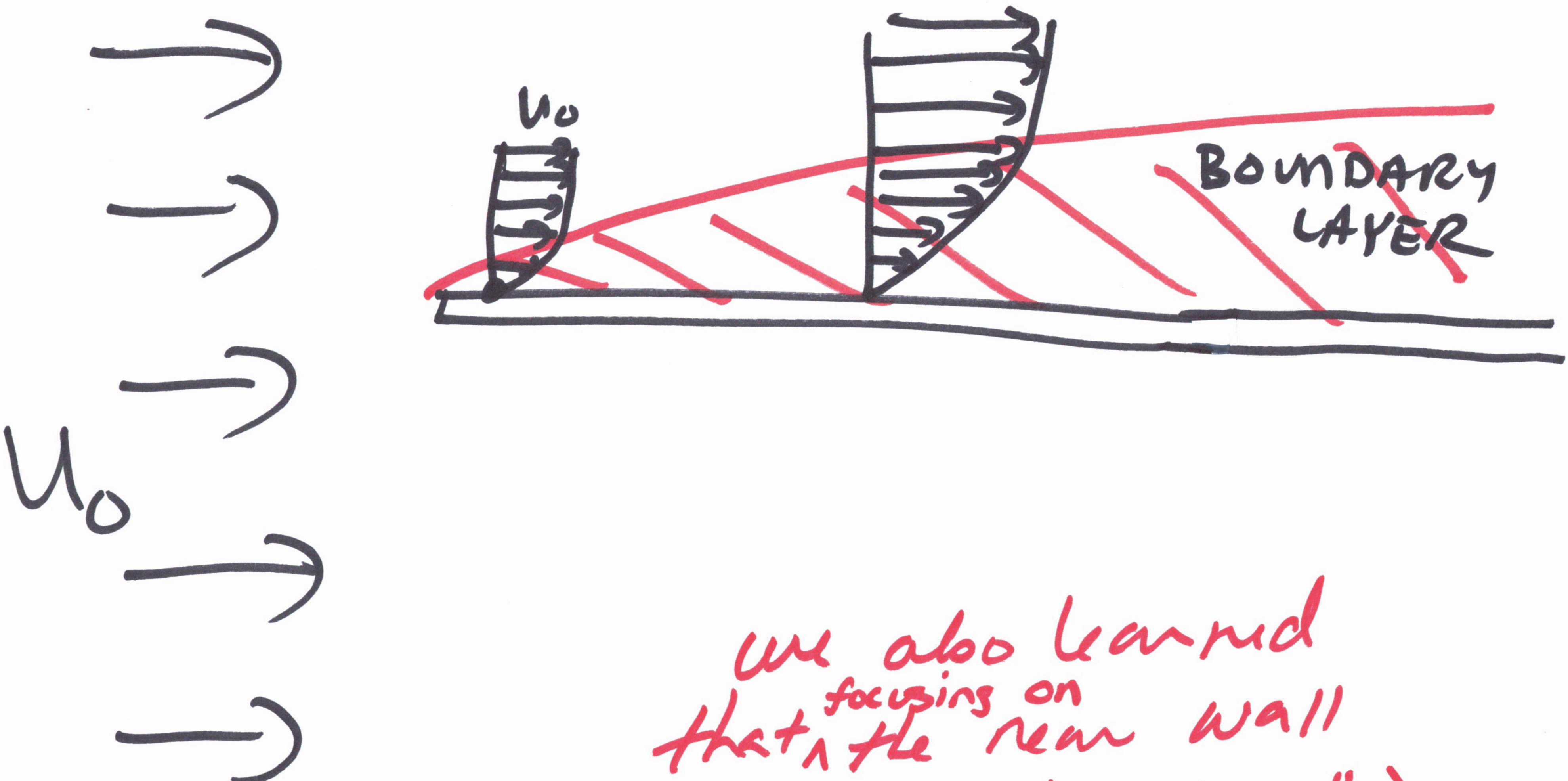


domain

$R_1 < r < R_2$

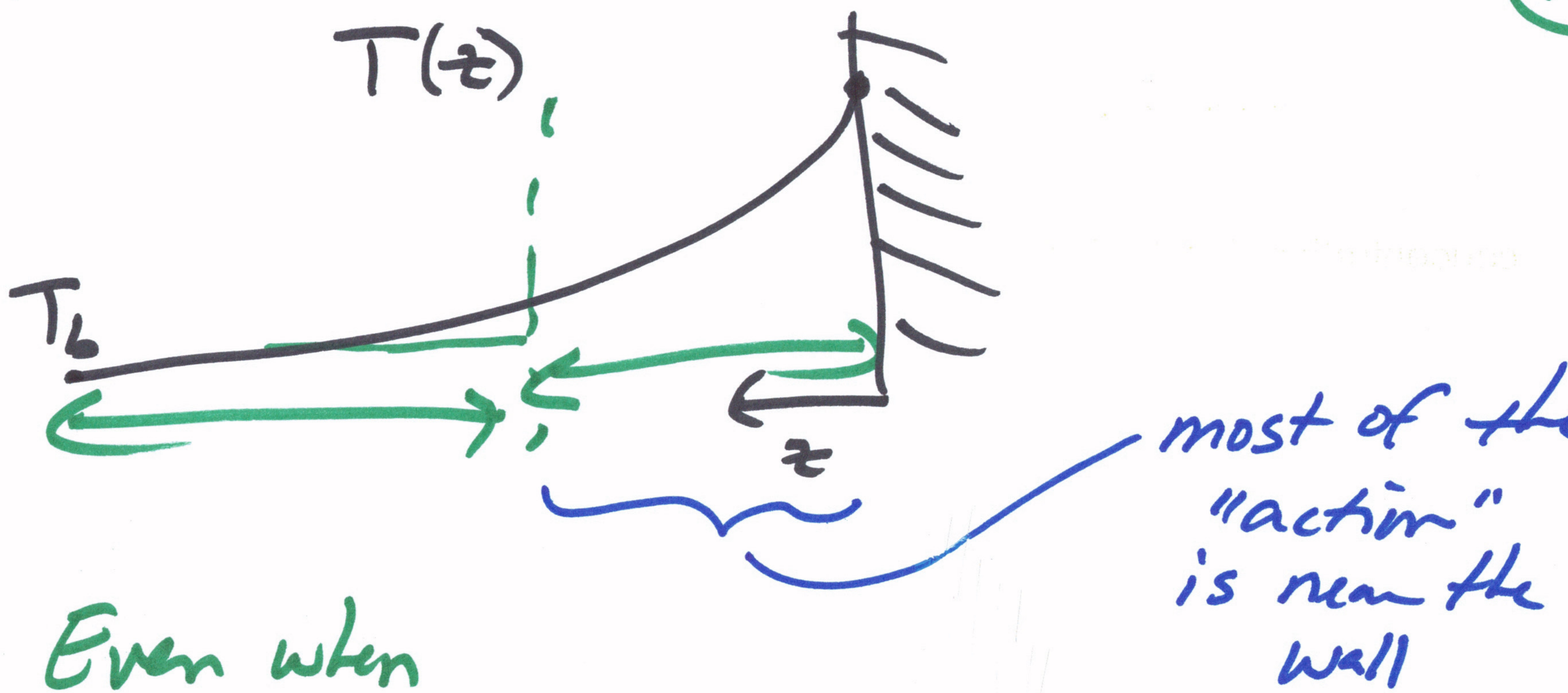
We Learn:
Look for
- domain, &
- BC!

FLUIDS:



we also learned that focusing on the near wall (or "near boundary") region is a successful modeling strategy...

HEAT TRANSFER:



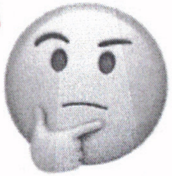
Even when $z \to \infty$ can be divided into "interesting" and "not much happening...

We also have notes (past experience) of things that have been successful: 1.4

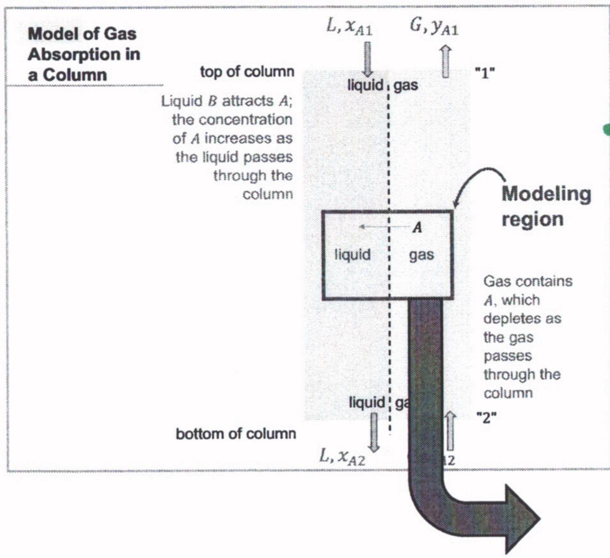
Recurring Modeling Assumptions in Diffusion ("Classics")

- 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 ($N_{Az} = J_{Az}^*$); also c is approximately constant
- 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, $\underline{N}_A = -\underline{N}_B$. (coming)

②



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.

$$A + B \rightarrow AB$$

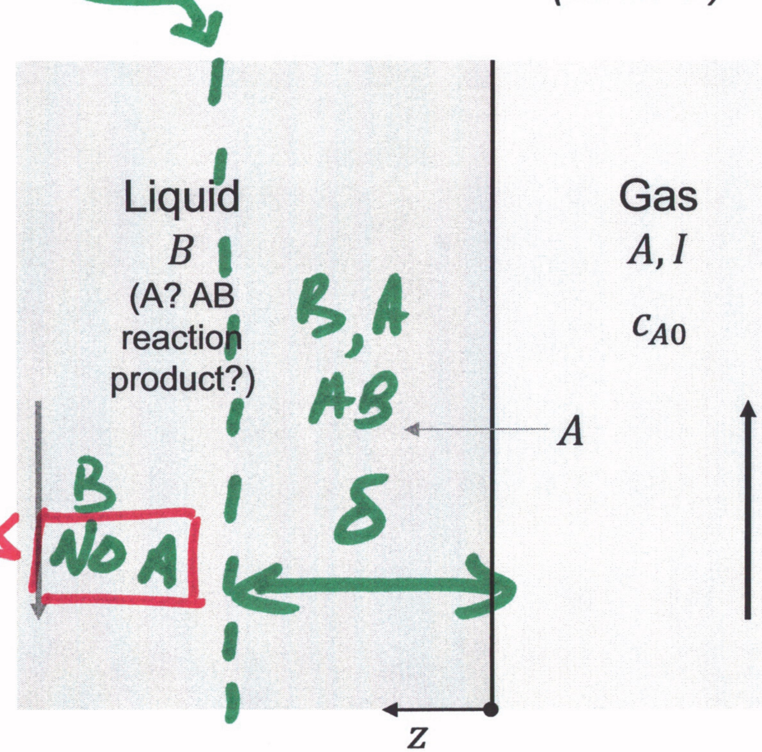
$$R_A = -k_1 c_A$$

How can we visualize (model) this happening?

What questions can we ask?

Thought: all A is gone at some point

(dilute A)



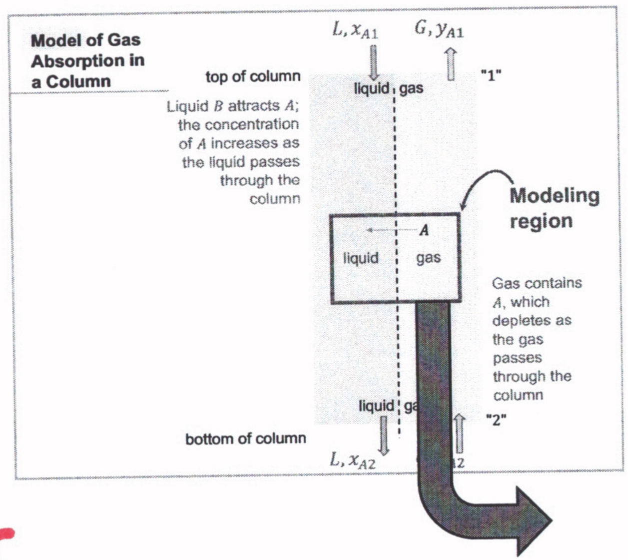
$0 \le z \le ?$

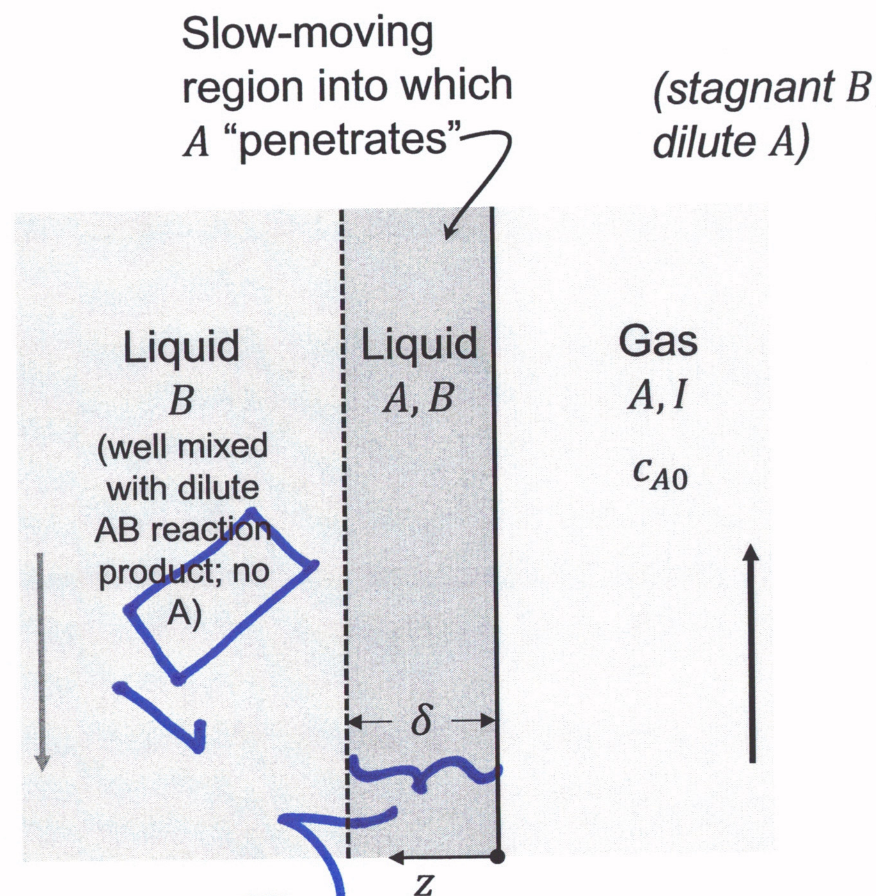
BC: $\begin{cases} z = 0, & x_A^* = x_A \\ z = \delta & x_A = 0 \leftarrow \text{all reacted} \end{cases}$

③

Example 5: Gas Absorption Column

Use a "*penetration model*"





Kinetics

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

$$A + B \rightarrow AB$$

$$R_A = -k_1 c_A$$

$0 \le z \le \delta$

Ready to "slash + burn"

C_A, $\underline{N}_A$, combined units

(4)

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

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

NOT ZERO!

YES

homo-geneous reaction

Step 3

1D diffusion

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

1D in z-dir

stagnant

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

STEP 1) Microscopic Species A mass bal:

$$-\frac{dN_{A,z}}{dz} + r_A = 0$$

$= -k_1 C_A$ (see earlier slide, CM3150)

STEP 2) Fick's Law of diffusion:

$$N_{A,z} = x_A N_{A,z} - c D_{AB} \frac{dx_A}{dz}$$

$$N_{A,z}(1 - \cancel{x_A}) = -c D_{AB} \frac{dx_A}{dz} = -D_{AB} \frac{dC_A}{dt}$$

ASSUME DILUTE

Solving:

$$-\frac{d}{dz}\left(N_{A,z}\right) - k_1 C_A = 0$$

$$-D_{AB}\frac{dC_A}{dz}$$

constant

$$D_{AB}\frac{d^2C_A}{dz^2} - k_1 C_A = 0$$

$$\boxed{\frac{d^2C_A}{dz^2} - \left(\frac{k_1}{D_{AB}}\right) C_A = 0}$$

BC: $z = 0 \quad C_A = C_A^*$

$z = \delta \quad C_A = 0$

Thinking back to differential eqns class:

$$y'' - a^2 y = 0$$

This is a 2nd order ODE with constant coefficients.

$y \rightarrow C_A$

$a \rightarrow \sqrt{k_1/D_{AB}}$

We look up the solution:

$$\boxed{C_A = C_1 \cosh\left(z\sqrt{\frac{k_1}{D_{AB}}}\right) + C_2 \sinh\left(z\sqrt{\frac{k_1}{D_{AB}}}\right)}$$

Apply BC; solve for C_1, C_2, DONE //