17&19 March 2021

17 March 2021
F. Morrison CM3120
Lecture VI, MODULE 3

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Classic 1D Steady Diffusion Summary

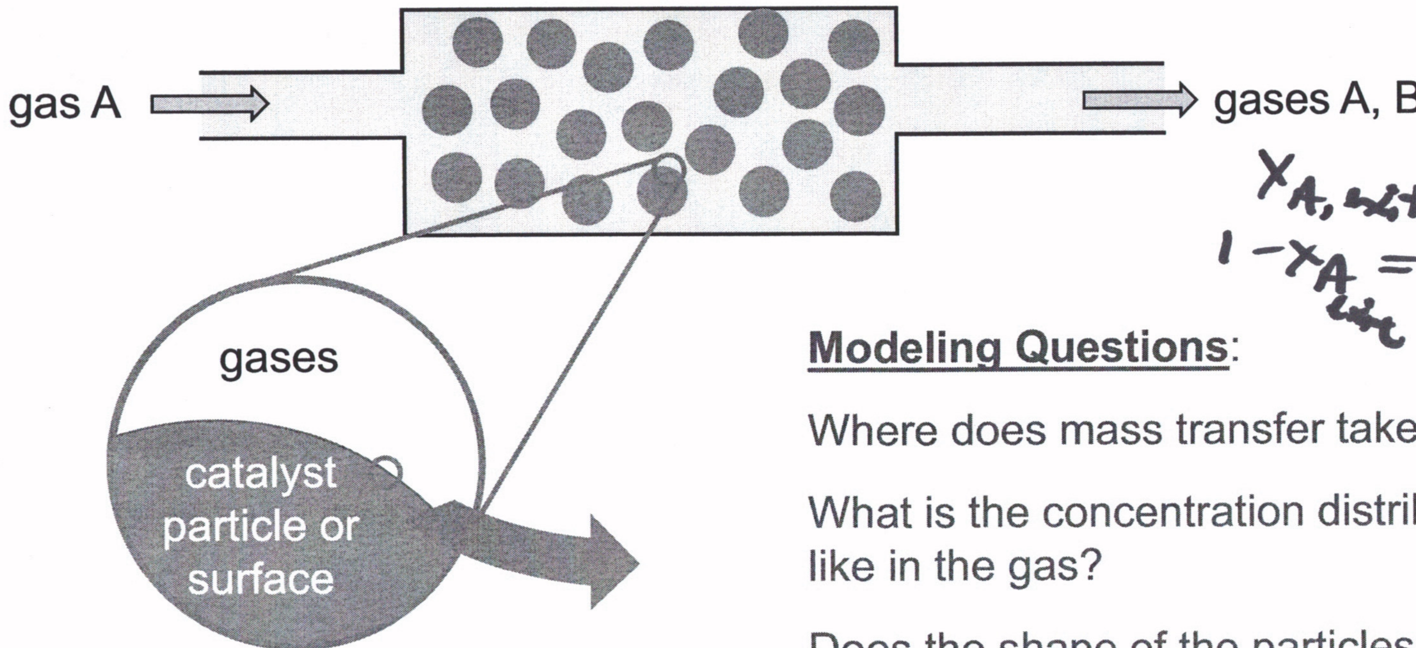
a. 1D rectangular mass transfer (evaporating tank, **Ex 1**)

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

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

3

Example 3: Heterogeneous catalysis



$x_{A,\text{exit}}$

$1 - x_{A,\text{exit}} = x_B$

Modeling Questions:

Where does mass transfer take place?

What is the concentration distribution like in the gas?

Does the shape of the particles matter?

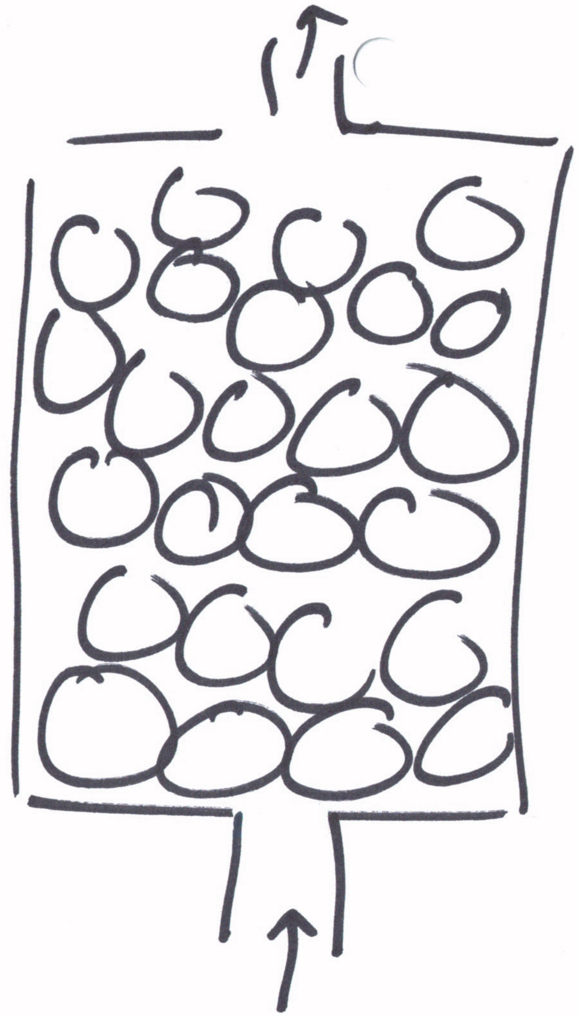
What is the impact of the overall (bulk) flow?

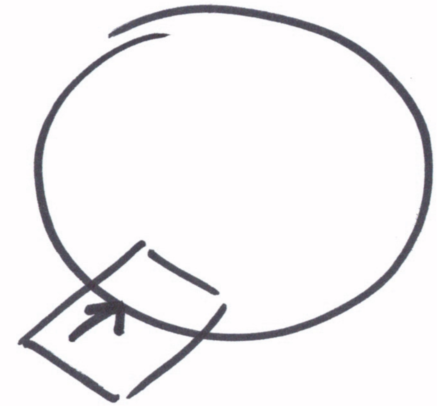
What should be our first modeling problem?

An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface in a reactor as shown. How might mass transfer affect the observed rate of reaction?

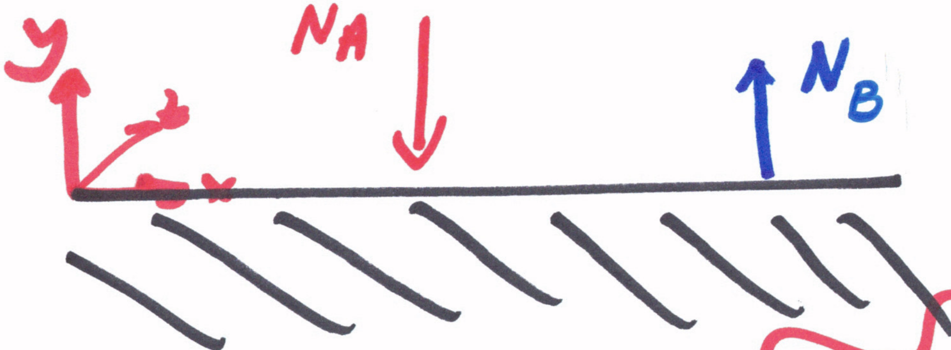
BSL2, p562

Thinking...





Gas A, B $2A \rightarrow B$



$N_A = (2)(-N_B)$

The ratio of A_{in} to B_{out} is 2:1

$0 \le y \le \infty$

What is x_A (position) in the gas?

What is N_A? constant? variable?

What is N_B?

ASIDE

Rxn: $2A \rightarrow B$

$$N_A = -2N_B$$

$$-\frac{1}{2}N_A = N_B$$

This can be confusing. This is a question of FLUX not stoichiometry

$$10 \text{ moles } A \longrightarrow \underbrace{5 \text{ moles } B}$$

$$N_A = \frac{10 \text{ moles } A}{\text{area time}} \qquad N_B = \frac{5 \text{ moles } B}{\text{Area} \cdot \text{time}}$$

$$10 \text{ moles } A \longrightarrow \boxed{RXR} \longrightarrow 5 \text{ moles } B$$

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

(5)

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

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

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

WRF 25-11

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

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

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

no homogeneous rxn

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

steady

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

flux is in y-dir alone

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

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

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

WRF 24-22

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

Fick's law of diffusion, Cartesian coordinates:

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

$-\frac{1}{2}N_A$
$= N_B$

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:

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

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microscopic species A bal

$$\frac{\partial N_{A,y}}{\partial y} = 0$$

$$\boxed{N_{A,y} = C_1}$$

Fick's Law:

$$N_{A,y} = x_A \underbrace{\left(N_{Ay} - \tfrac{1}{2} N_{Ay}\right)}_{\frac{1}{2} N_{A,y}} - c\mathcal{D}_{AB} \frac{\partial x_A}{\partial y}$$

(See HW3 Prob 10)

$$N_A \left(1 - \tfrac{1}{2} x_A\right) = -c\mathcal{D}_{AB} \frac{dx_A}{dy}$$

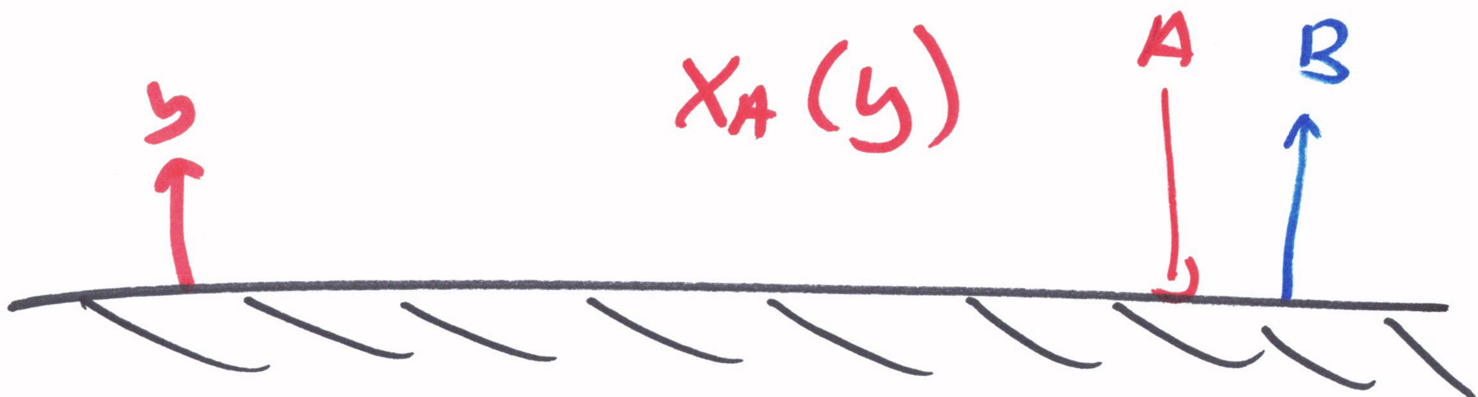
$\therefore$ continue

X_A is function of y

integrate with respect to y
(will add "c_1", integration constant)

(HW3)

BC:

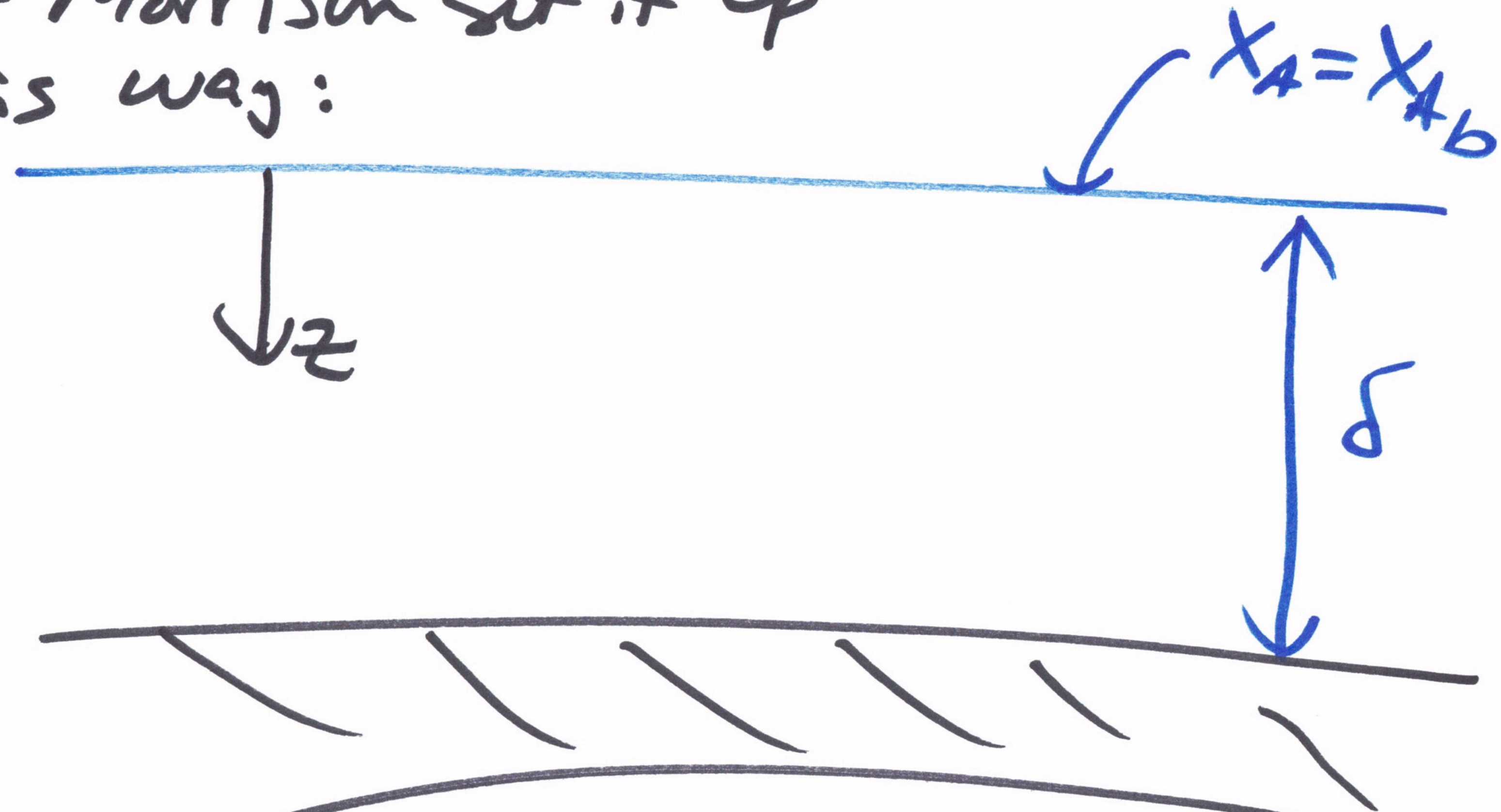


$y = \infty \quad X_A = X_{A\,bulk}$

$y = 0 \quad X_A = 0$

(I set it up differently in HW3)

What are the boundary conditions? Dr Morrison set it up this way:



$z = 0 \quad x_A = x_{A,bulk}$

$z = \delta \quad x_A = 0$