

**It's week 7. Next week is Week 8.
Exam 3: Week 9 (after break)**

**Homework 3A:
Finish Week 6**

HW3

Michigan Technological University
Chemical Engineering

CM3120 Transport/Unit Ops 2
Unsteady State Heat Transfer and Diffusion.

HW3a: Unsteady heat transfer (finish week 6)

- Compare the characteristic time we used in laminar/turbulent flow (momentum transport, non-dimensionalization of the microscopic momentum balance) and what we used in unsteady state heat transport (part of the Fourier number). What is the ratio? What does it mean in models we develop for this number to be large or small?
- A large, iron structure (approximate dimensions 3m x 3m x 3m, iron) initially with a uniform temperature of 100°C is exposed to outside air conditions (air temperature = 25°C, heat transfer coefficient = $2.0 \times 10^4 \text{ W/m}^2\text{K}$). What is the wall temperature after 35 minutes?
- Estimate the temperature at the center of a one-inch diameter solid brass sphere thirty seconds into being subjected to the following treatment: first the sphere is held in a bath and allowed to equilibrate at 10°C; subsequently the sphere is submerged into a vigorously stirred bath at constant temperature 85°C. Assume a heat transfer coefficient of $2300 \text{ W/m}^2\text{K}$. Answer: 84.6°C or 85°C based on the assumptions made and sig figs.
- Stretch: Using Excel, MATLAB, or software of your choosing, create the Heisler chart for the temperature at the center of a sphere as a function of time and Biot number (https://chem.mtu.edu/cm3120/unitops/3120/Heisler_chart_for_week_2019.pdf). Answer: see Appendix F. See TA with questions.
- If we expose a hot dog to the outside winter temperature, it will cool off. How fast it will cool off depends on the wind, how cold it is, and perhaps other factors. Model this process and indicate how you will come to an estimate of how long it will take for a hot dog initially at -200°F to cool to a lukewarm -100°F . Find realistic values for parameters you will need. Answer: Will depend a bit on your assumptions. Our answer was $\approx 1s$.

**Homework 3B:
Finish Week 8**

HW3

Michigan Technological University
Chemical Engineering

HW3b: Intro to mass transfer (finish week 8)

- Show that the following relationships for the various versions of the species mass/molar fluxes hold (do not assume Fick's law to show the equalities)
 - $\bar{v}_A + \bar{v}_B = v^*$
 - $\bar{v}_A + \bar{v}_B = v^*$
 - $\bar{v}_A + \bar{v}_B = v^*$
 - $\bar{v}_A + \bar{v}_B = v^*$

In a sentence or two, what are the differences among the various fluxes in the question above? Why have we chosen to use such a variety of nomenclature?

- Species A (gas) is diffusing through stagnant species B (also a gas) at steady state. The situation may be considered to be one-dimensional (1D) diffusion. The steady state flux of species A is $5.0 \times 10^{-8} \text{ kmol A/m}^2\text{s}$. At one point in the diffusion space, the concentration of A is 0.0008 kmol/m^3 and the concentration of B is 0.0016 kmol/m^3 . What is your estimate of the individual velocities of species A and B along the direction of mass transfer? What is the average molar velocity? Answer: $v^* = 0.0012 \text{ m/s}$.
- Species A (gas) and species B (also a gas) form a binary mixture in which steady equimolar counter diffusion is occurring (see p499 of WHF, posted at https://pages.mtu.edu/~chem3120/unitops/3120/WHF2019_page499-500.pdf). The situation may be considered to be one-dimensional (1D) diffusion. The steady state flux of species A is $5.0 \times 10^{-8} \text{ kmol A/m}^2\text{s}$. At one point in the diffusion space, the concentration of A is 0.0008 kmol/m^3 and the concentration of B is 0.0016 kmol/m^3 . What is your estimate of the individual velocities of species A and B along the direction of mass transfer? What is the average molar velocity? If it is water and B is nitrogen, what is the mass-average velocity? Answer: $v_x = -4.6 \times 10^{-10} \text{ m/s}$; $v_x^* = 0$. Comment on the difference.
- Secum album (an important blood protein) is a long-chain polymer that takes on a roughly spherical conformation. If we think of the diffusion of secum albumin as similar to the diffusion of a sphere moving through a solvent (water), we can estimate the size of the molecule. The measured diffusion coefficient of secum albumin is $5.94 \times 10^{-10} \text{ cm}^2/\text{s}$ at 293K. Based on this measured diffusivity, what is the radius of the sphere? Answer: $r = 7.2 \mu\text{m}$.
- A hemispherical drop of liquid is evaporating through a film of air of thickness δ . The temperature and air concentration distribution in the film is shown in the figure below. The temperature in the film is not constant but varies as $T(r)/T(R_0) = (T(R_0)/T(R_0))^{1/2}$; note that this means that both the diffusivity D_{AB} and the concentration $c = P/AT$ are a function of position through their temperature dependences. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air; you may assume that the diffusivity varies with temperature as follows: $D_{AB}(T)/D_{AB,1} = (T/T_1)^{1.75}$

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Diffusion and Mass Transfer

Michigan Technological University
Chemical Engineering

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer in MIXTURES

Professor Faith A. Morrison
Department of Chemical Engineering
Michigan Technological University
www.chem.mtu.edu/~fmorrison/cm3120/unitops125.html

It turns out that there are many interesting and applicable problems we can address readily with this form of the species mass balance.

Microscopic species mass balance in a frame

$$\frac{\partial}{\partial t} (\rho c_A) + \nabla \cdot (\rho c_A \mathbf{v}_A) = -\nabla \cdot \mathbf{J}_A + \dot{r}_A$$

Let's jump in!

We'll do a "Quick Start" and get into some examples and return to the "why" of it all a bit later.

QUICK START
(to problem solving)

Continuing...

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Film model of mass transfer QUICK START

Last time, we did this second problem:

The primary goal is to grow our ability to troubleshoot engineering problems.

EXAMPLE 2

Let's do another problem

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). What is the rate of evaporation and how does the water concentration vary in the gas?

Ver 1

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Film model of mass transfer QUICK START

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

We invented the "film model"

Ver 2

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Film model of mass transfer

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

The Film Model of mass transfer Ver 2

②

Equation of Species Mass Balance in Terms of Concentration

③

Microscopic species A mass balance

④

Fick's Law of Diffusion

Microscopic species A mass balance ③

- steady
- no rxn
- θ, ϕ symmetry (see p2)

$$0 = \frac{1}{r^2} \frac{d}{dr} (r^2 N_{Ar})$$

$$\frac{d\Phi}{dr} = 0$$

$$r^2 N_{Ar} = \Phi = C_1$$

$$N_{Ar} = \frac{C_1}{r^2}$$

Fick's Law of Diffusion ④

- constant D
- steady state
- θ, ϕ symmetric

$$N_{Ar} = x_A N_{Ar} - c D_{As} \frac{dx_A}{dr}$$

...
Solve

assume const
 $c = \frac{P}{RT} = \text{const}$

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Film model of mass transfer

Ver 2

Assumptions:

- Uniform film surrounds droplet
- Ideal gas
- Constant temperature and pressure

QUICK START

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

Ver 2

Solution:

$x_A(r)$

$$\frac{1 - x_{A1}}{1 - x_{A2}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right) \left(\frac{\frac{1}{R_1} - \frac{1}{r}}{\frac{1}{R_1} - \frac{1}{R_2}} \right)$$

Open: How would we "answer the question" in this problem?

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QUICK START

↻

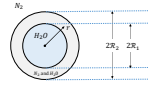
We can now explore these assumptions, and modify, if needed, for more complex problems.

Ver 2

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

Assumptions:

- Uniform film surrounds droplet
- Ideal gas
- Constant temperature and pressure



Solution:

$x_A(r)$

$$\frac{1 - x_A}{1 - x_{A1}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right)^{\left(\frac{\frac{1}{R_1} \frac{1}{r}}{\frac{1}{R_1} \frac{1}{R_2}} \right)}$$

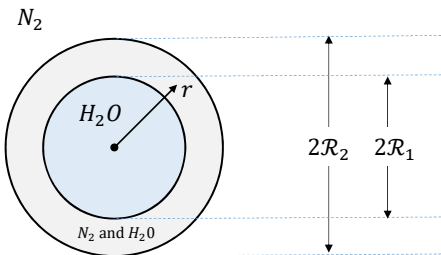
Ver 2

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QUICK START

Film model of mass transfer

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.



Assumptions:

- Uniform film
- Ideal gas
- Constant pressure
- Constant temperature

Let's Interrogate the problem.

How good are these assumptions?

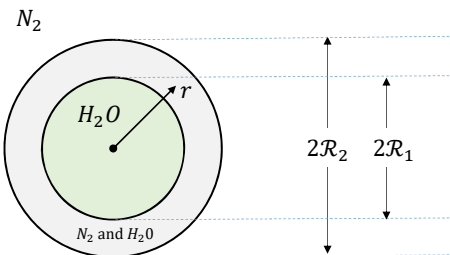
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Film model of mass transfer (more complex) QUICK START

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet?

Note: *not* isothermal



$\Delta \hat{h}_{\text{vap}} \neq 0$

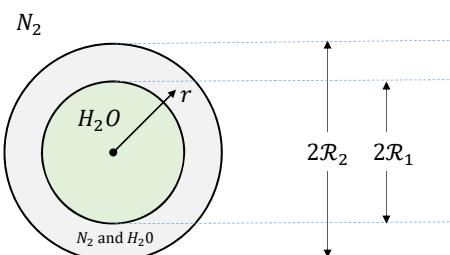
Ver 3

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Film model of mass transfer (more complex) QUICK START

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet?

Note: *not* isothermal



$\Delta \hat{h}_{\text{vap}} \neq 0$

What does changing temperature impact?

How do we modify the model?

Ver 3

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Film model of mass transfer (more complex)

Where did we assume "isothermal"?

Example 2 A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

The Film Model of mass transfer

Ver 2

Equation of Species Mass Balance in Terms of Φ

Microscopic species A mass balance

- steady
- no rxn
- Φ symmetry

(See p.2)

$$0 = \frac{1}{r^2} \frac{d}{dr} (r^2 N_{Ar})$$

$$\frac{d\Phi}{dr} = 0$$

$$\Rightarrow N_{Ar} = \Phi = C_1$$

$$N_{Ar} = \frac{C_1}{r^2}$$

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$$N_{Ar} = \frac{C_1}{r^2}$$

Flux is Limit of Diffusion

- constant T
- Φ symmetric

assume const

$$N_{Ar} = x_A N_{Ar} - c D_{A0} \frac{dx_A}{dr}$$

Solve

$$c = \frac{N}{V} = \frac{P}{RT} = \text{const}$$

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Film model of mass transfer (more complex)

Where did we assume "isothermal"?

When we integrated to obtain $x_A(r)$.

Example 2 A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

The Film Model of mass transfer

Ver 2

Equation of Species Mass Balance in Terms of Φ

Microscopic species A mass balance

- steady
- no rxn
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(See p.2)

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Solve

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Film model of mass transfer (more complex) QUICK START

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air; you may assume that the diffusivity varies with temperature as follows:

$$D_{AB}(T)/D_{AB,1} = (T/T_1)^{3/2}$$

Note: *not* isothermal HW3, problem 12 (stretch)

Ver 4

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Film model of mass transfer (more complex) QUICK START

Ver 4

Assumptions:

- Uniform film surrounds droplet
- Ideal gas
- Temperature follows power law
- Diffusivity follows power law
- Pressure is constant

Solution:

$x_A(r)$

$$\frac{1 - x_{A1}}{1 - x_{A2}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right) \left(\frac{\mathcal{R}_1^{1+n/2} r^{1+n/2}}{\mathcal{R}_1^{1+n/2} \mathcal{R}_2^{1+n/2}} \right)$$

Note: *not* isothermal HW3, problem 12 (stretch)

Ver 4

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The primary goal is **to grow our ability to troubleshoot engineering problems.**

QUICK START

Let's do another problem, more complex

EXAMPLE 3

Example 3: Heterogeneous catalysis

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

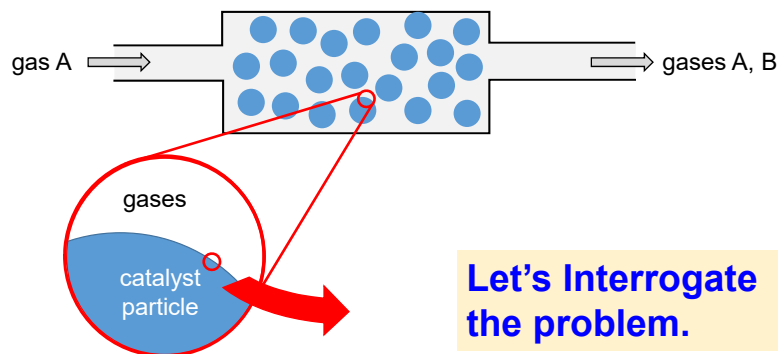
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Film model of mass transfer (more complex)

QUICK START

Example 3



Example 3: Heterogeneous catalysis

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?**

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QUICK START

Let's Interrogate the problem.

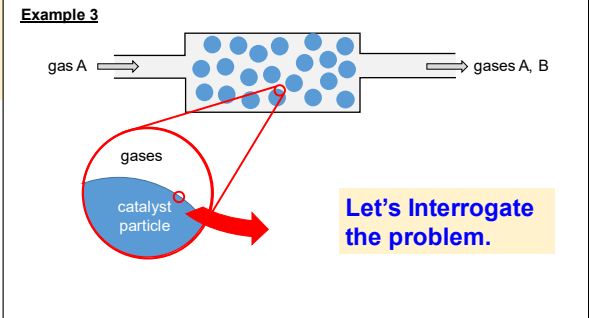
*What is the geometry?
What does it affect?*

How does diffusion affect how fast the chemical transformation takes?

How would diffusion take place (look for sources, sinks)

What is the governing physics?

Example 3



Let's Interrogate the problem.

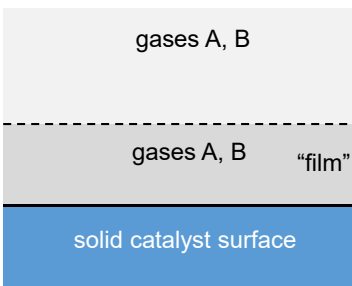
Example 3: Heterogeneous catalysis
An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface in a reactor as shown. *How might mass transfer affect the observed rate of reaction?*

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QUICK START

Film model of mass transfer (more complex)

Example 3: Heterogeneous catalysis
An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film $x_A(z)$ and the flux of product B away from the surface.



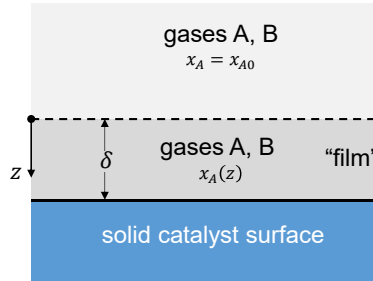
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Film model of mass transfer (more complex)

QUICK START

Example 3: Heterogeneous catalysis

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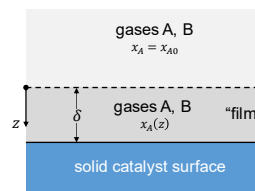
- Deploy the "film model"
- It has become a way of thinking about diffusion in some circumstances

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QUICK START

Example 3: Heterogeneous catalysis

An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film $x_A(z)$ and the flux of product B away from the surface.



SOLVE

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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.

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

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

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

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

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

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

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

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

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

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Fick's Law of Diffusion in terms of Combined Molar Flux \underline{N}_A

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

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

Fick's law of diffusion, Cartesian coordinates: $\left(\begin{matrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{matrix}\right)_{xyz} = \left(\begin{matrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB} \frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB} \frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{matrix}\right)_{xyz}$

Fick's law of diffusion, cylindrical coordinates: $\left(\begin{matrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{matrix}\right)_{r\theta z} = \left(\begin{matrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{matrix}\right)_{r\theta z}$

Fick's law of diffusion, spherical coordinates: $\left(\begin{matrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{matrix}\right)_{r\theta\phi} = \left(\begin{matrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{matrix}\right)_{r\theta\phi}$

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QUICK START

SOLUTION:

Example 3: Heterogeneous catalysis
 An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film ($x_A(z)$) and the flux of product B away from the surface.

See hand slides for start;
 solution assigned in HW4

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Film model of mass transfer (more complex)

Assumptions:

- Fast, irreversible reaction at surface
- Diffusion through film at surface limits rate of reaction
- Steady state
- Constant T, P

Example 3: Heterogeneous catalysis

An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film ($x_A(z)$) and the flux of product B away from the surface.

Solution:

$$x_A(z)$$

$$\left(1 - \frac{1}{2} x_A\right) = \left(1 - \frac{1}{2} x_{A0}\right)^{(1-z/\delta)}$$

Open: How would we "answer the question" in this problem?

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Introduction to Diffusion and Mass Transfer in Mixtures
QUICK START

Recurring Modeling Assumptions in Diffusion

- 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, $\underline{N}_A = 0$.
- If A diffuses through stagnant B , $\underline{N}_B = 0$.
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction converts it to one mole of B , then at steady state $-0.5\underline{N}_A = \underline{N}_B$.
- Because diffusion is slow, we can make a quasi-steady-state assumption
- Homogeneous reactions appear in the mass balance; heterogeneous reactions appear in the boundary conditions
- If a binary mixture of A and B are undergoing steady equimolar counter diffusion, $\underline{N}_A = -\underline{N}_B$. (coming)
-
-

25
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We have been performing a "Quick Start,"

And have found the **combined molar flux** formulation useful.

It turns out that there are many interesting and applicable problems we can address readily with **this** form of the species mass balance.

Microscopic species A mass balance—Five forms	
In terms of mass flux and mass concentrations	$\rho \left(\frac{\partial \omega_A}{\partial t} + \mathbf{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \mathbf{j}_A + r_A$ $= \rho D_{AB} \nabla^2 \omega_A + r_A$
In terms of molar flux and molar concentrations	$c \left(\frac{\partial x_A}{\partial t} + \mathbf{v} \cdot \nabla x_A \right) = -\nabla \cdot \mathbf{j}_A + R_A$ $= c D_{AB} \nabla^2 x_A + R_A$
In terms of combined molar flux and molar concentrations	$\frac{dc_A}{dt} = -\nabla \cdot \mathbf{N}_A + R_A$

Microscopic species mass balance in terms of combined molar flux \underline{N}_A

Let's jump in!

We'll do a "Quick Start" and get into some examples and return to the "why" of it all a bit later.

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There are times it is not useful. We need to go back and discuss *how/why/when* this all works.

Various forms of Fick's Law (and the species mass balances that employ them)

<p>Mass flux</p> $j_A = -\rho D_{AB} \nabla \omega_A$	<p>Molar flux</p> $J_A = -c D_{AB} \nabla x_A$	<p>Combined molar flux</p> $N_A = x_A(N_A + N_B) - c D_{AB} \nabla x_A$
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FRONT

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Now, Cycling Back:

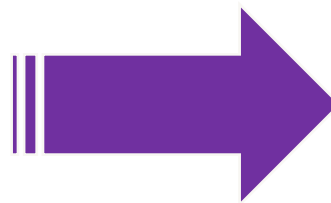
Diffusion and Mass Transfer

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer

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