TRANSPORT PHENOMENA II (0905342)

# 05- STEADY STATE APPLICATIONS: SOLIDS

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# Outline

- Diffusion through solids
- Diffusion through gases
- Diffusion through liquids

# Species Equation of Continuity: Various Coordinate Systems

- Rectangular coordinate system

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

- Cylindrical coordinate system

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

- Spherical coordinate system

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

# Fick's Second Law in Various Coordinate Systems

- Rectangular coordinate system

$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2}\right]$$

- Cylindrical coordinate system

$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c_A}{\partial \theta^2} + \frac{\partial^2 c_A}{\partial z^2}\right]$$

- Spherical coordinate system

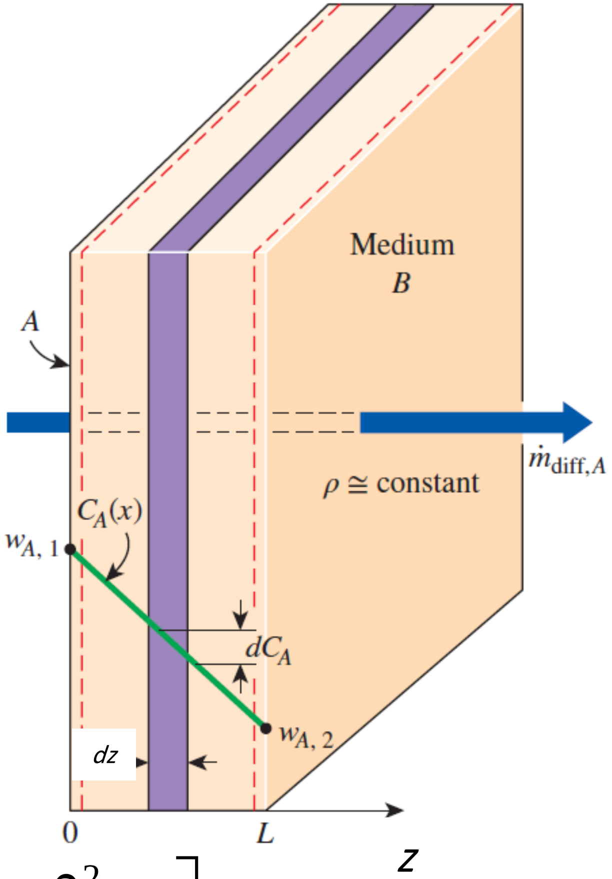
$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial c_A}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 c_A}{\partial \phi^2}\right]$$

# Diffusion in Solids Following Fick's Law

- Diffusion following Fick's law (does not depend on the structure of the solid)
- This situation is met, when the solute dissolves and forms a homogeneous solution with the solid.
  - Steady-state diffusion through a solid slab (planar surface).
  - Steady-state diffusion through a hollow cylindrical surface.
  - Steady-state diffusion through a spherical cavity.
- Consider a solid plane wall (medium B) of area A, thickness L, and density ρ.
  - The wall is subjected on both sides to different concentrations of a species A to which it is permeable.
  - The boundary surfaces at $x = 0$ and $x = L$ are located within the solid adjacent to the interfaces, and the concentration is constant at all times.
  - The concentration of species A in the wall varies in the x-direction only.
  - Therefore, mass transfer through the wall in this case can be modeled as steady and one-dimensional.

# Steady-State Diffusion Through a Solid Slab (Planar Surface)

- Consider a solid plane wall (medium B) of area A, thickness L, and density ρ.
  - The wall is subjected on both sides to different concentrations of a species A to which it is permeable.
  - The boundary surfaces at x = 0 and x = L are located within the solid adjacent to the interfaces, and the concentration is constant at all times.
  - The concentration of species A in the wall varies in the x-direction only.
  - Therefore, mass transfer through the wall in this case can be modeled as steady and one-dimensional.
- Since the diffusion is through the solid the bulk term is set to zero in solids




$$N_A = -D_{AB}\frac{dc_A}{dz} + \frac{c_A}{c_T}(N_A + N_B)$$

$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2}\right]$$

$$\frac{\partial^2 c_A}{\partial z^2} = 0$$

$$\text{B.C.1: } c_A(z = 0) = c_{A,1}$$

$$\text{B.C.1: } c_A(z = L = z_2 - z_1) = c_{A,2}$$

The well-posed formulation for diffusion through a solid planar wall

$$c_A(z) = \left(c_{A,2} - c_{A,1}\right)\frac{z}{L} + c_{A,1}$$

Concentration profile

$$N_A = D_{AB}\frac{c_{A1} - c_{A2}}{z_2 - z_1} = D_{AB}\frac{c_{A1} - c_{A2}}{L}$$

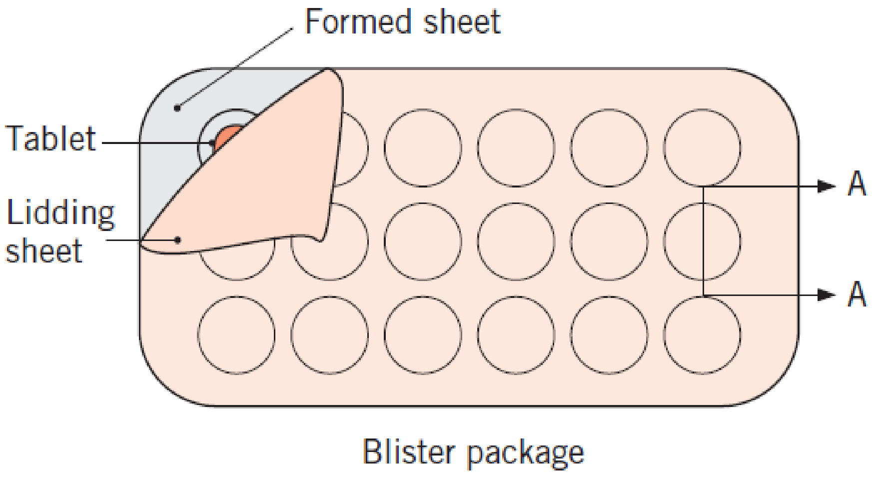
Shell balance yields constant flux and $D_{AB}$ is assumed constant

- Density and the diffusion coefficient of the wall are assumed to be nearly constant. This assumption is reasonable.
- when a small amount of species A diffuses through the wall and thus the concentration of A is small.
- Species A can be a gas, a liquid, or a solid.
- The wall can be a plane layer of a liquid or gas provided that it is stationary.
- Many times if the curvature of a sphere or cylinder is not that large we may approximate it as a planar wall.

## Example 14.3

The efficacy of pharmaceutical products is reduced by prolonged exposure to high temperature, light, and humidity. For water vapor–sensitive consumer products that are in tablet or capsule form, and might be stored in humid environments such as bathroom medicine cabinets, *blister packaging* is used to limit the direct exposure of the medicine to humid conditions until immediately before its ingestion.

Consider tablets that are contained in a blister package composed of a flat *lidding sheet* and a second, *formed sheet* that includes troughs to hold each tablet. The formed sheet is $L = 50$ µm thick and is fabricated of a polymer material. Each trough is of diameter $D = 5$ mm and depth $h = 3$ mm. The lidding sheet is fabricated of aluminum foil. The binary diffusion coefficient for water vapor in the polymer is $D_{AB} = 6 \times 10^{-14}$ m$^2$/s while the aluminum may be assumed to be impermeable to water vapor. For molar concentrations of water vapor in the polymer at the outer and inner surfaces of $C_{A,s1} = 4.5 \times 10^{-3}$ kmol/m$^3$ and $C_{A,s2} = 0.5 \times 10^{-3}$ kmol/m$^3$, respectively, determine the rate at which water vapor is transferred through the trough wall to the tablet.



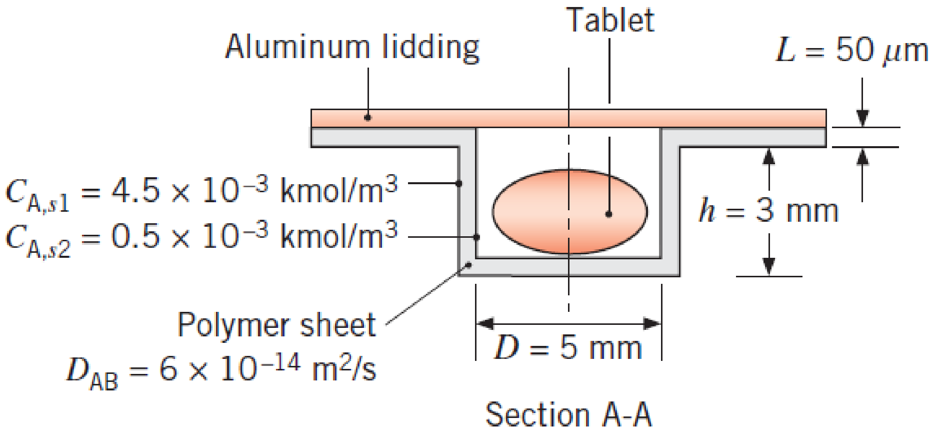

From Incopera

## SOLUTION

***Known:*** Molar concentrations of water vapor at the inner and outer surfaces of a polymer sheet and trough geometry.

***Find:*** Rate of water vapor molar diffusive transfer through the trough wall.

***Schematic:***




***Assumptions:***

1. Steady-state, one-dimensional conditions.
2. Stationary medium.
3. No chemical reactions.
4. Polymer sheet is thin relative to the dimensions of the trough, and diffusion may be analyzed as though it occurs through a plane wall.

***Analysis:*** The total water vapor transfer rate is the summation of the transfer rate through the cylindrical walls of the trough and the bottom, circular surface of the trough. From Equation 14.54 we may write

$$N_{A,x} = \frac{D_{AB} A}{L}(C_{A,s1} - C_{A,s2}) = \frac{D_{AB}}{L}\left(\frac{\pi D^2}{4} + \pi D h\right)(C_{A,s1} - C_{A,s2})$$

Hence

$$N_{A,x} = \frac{6 \times 10^{-14}\ \text{m}^2/\text{s}}{50 \times 10^{-6}\ \text{m}}\left[\frac{\pi(5 \times 10^{-3}\ \text{m})^2}{4} + \pi(5 \times 10^{-3}\ \text{m})(3 \times 10^{-3}\ \text{m})\right]$$

$$\times (4.5 \times 10^{-3} - 0.5 \times 10^{-3})\ \text{kmol/m}^3$$

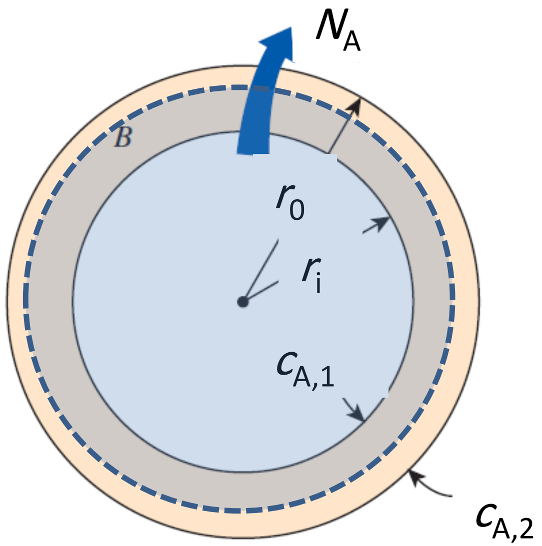
$$= 0.32 \times 10^{-15}\ \text{kmol/s} \qquad \triangleleft$$

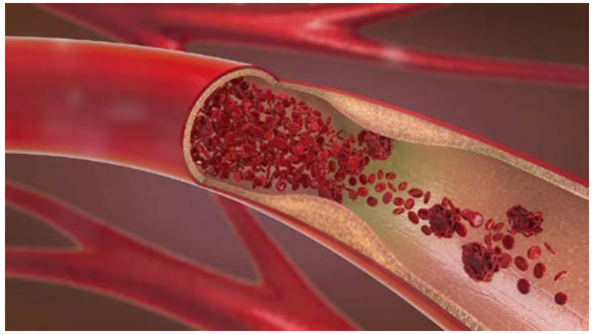
***Comments:***

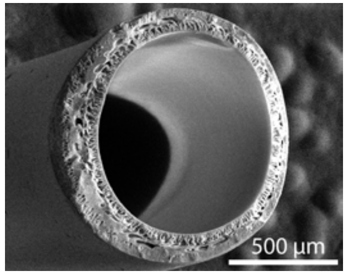
1. The mass diffusion rate of water vapor is $n_{A,x} = \mathcal{M}_A N_{A,x} = 18\ \text{kg/kmol} \times 0.32 \times 10^{-15}$ kmol/s $= 5.8 \times 10^{-15}$ kg/s.
2. The *shelf life* of the medicine is inversely proportional to the rate at which water vapor is transferred through the polymer sheet. Shelf life may be extended by increasing the thickness of the sheet, resulting in increased cost of the package. Specification of materials for use in blister packaging involves tradeoffs between shelf life, cost, formability, and recyclability of the polymer material.

# Steady One Dimensional Diffusion Through Nonreacting Cylindrical Layer

- Consider a solid hollow cylinder (medium B) of area A, thickness L, and density ρ.
  - The wall is subjected on both sides to different concentrations of a species A to which it is permeable.
  - The boundary surfaces at $r = r_i$ and $r = r_0$ are located within the solid adjacent to the interfaces, and the concentration is constant at all times.
  - The concentration of species A in the wall varies in the r-direction only.
  - Therefore, mass transfer through the wall in this case can be modeled as steady and one-dimensional.






$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c_A}{\partial \theta^2} + \frac{\partial^2 c_A}{\partial z^2}\right]$$

$$\frac{\partial}{\partial r}\left( r \frac{\partial c_A}{\partial r} \right) = 0$$

$$\text{B.C.1: } c_A(r = r_i) = c_{A,i}$$

$$\text{B.C.1: } c_A(r = r_0) = c_{A,0}$$

The well-posed formulation for diffusion through a hollow cylinder

$$c_A(r) = c_{A,i} - \frac{c_{A,i} - c_{A,0}}{\ln \frac{r_0}{r_i}} \ln \frac{r}{r_i}$$

Concentration profile

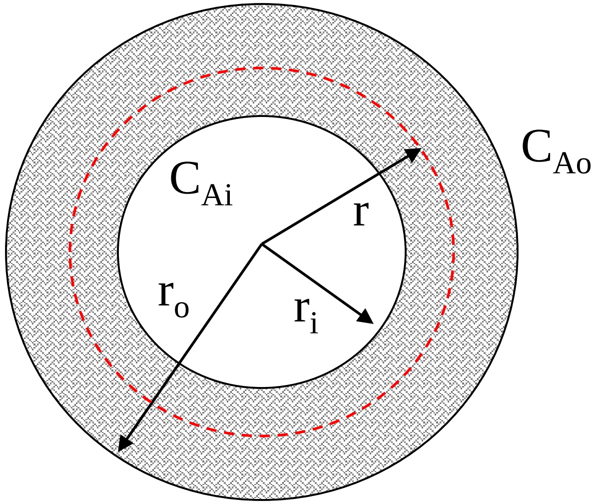
$$\overline{N}_A = -2\pi r L D_{AB} \frac{dc_A}{dr} = 2\pi L D_{AB} \frac{c_{A,i} - c_{A,0}}{\ln \frac{r_0}{r_i}}$$

Shell balance yields constant rate and $D_{AB}$ is assumed constant

- Density and the diffusion coefficient of the shell are assumed to be nearly constant. This assumption is reasonable.
- when a small amount of species A diffuses through the shell and thus the concentration of A is small.
- Species A can be a gas, a liquid, or a solid.
- Many times if the curvature of a sphere or cylinder is not that large we may approximate it as a planar wall.

# Steady One Dimensional Diffusion Through Nonreacting Spherical Layer

- Consider a solid hollow sphere (medium B) of of radius $r_0$.
  - The wall is subjected on both sides to different concentrations of a species A to which it is permeable.
  - The boundary surfaces at $r = r_i$ and $r = r_0$ are located within the solid adjacent to the interfaces, and the concentration is constant at all times.
  - The concentration of species A in the wall varies in the r-direction only.
  - Therefore, mass transfer through the wall in this case can be modeled as steady and one-dimensional.




$$\frac{\partial c_A}{\partial t} = D_{AB}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial c_A}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 c_A}{\partial\phi^2}\right]$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_A}{\partial r}\right) = 0$$

$$\text{B.C.1: } c_A(r = r_i) = c_{A,i}$$

$$\text{B.C.1: } c_A(r = r_0) = c_{A,0}$$

The well-posed formulation for diffusion through a hollow sphere (shell)

$$x_A(r) = \frac{x_{A,s1} - x_{A,s2}}{1/r_1 - 1/r_2}\left(\frac{1}{r} - \frac{1}{r_2}\right) + x_{A,s2}$$

$$c_A(r) = c_{A,0} + \frac{c_{A,i} - c_{A,0}}{\frac{1}{r_i} - \frac{1}{r_0}}\left(\frac{1}{r} - \frac{1}{r_0}\right)$$

Concentration profile

$$\overline{N}_A = 4\pi r_i r_0 D_{AB} \frac{c_{A,i} - c_{A,0}}{r_i - r_0}$$

Shell balance yields constant rate and $D_{AB}$ is assumed constant

- Density and the diffusion coefficient of the shell are assumed to be nearly constant. This assumption is reasonable.
- when a small amount of species A diffuses through the shell and thus the concentration of A is small.
- Species A can be a gas, a liquid, or a solid.
- Many times if the curvature of a sphere or cylinder is not that large we may approximate it as a planar wall.

## EXAMPLE 14–5 Diffusion of Hydrogen Through a Spherical Container

Pressurized hydrogen gas is stored at 358 K in a 4.8-m-outer-diameter spherical container made of nickel (Fig. 14–23). The shell of the container is 6 cm thick. The molar concentration of hydrogen in the nickel at the inner surface is determined to be 0.087 kmol/m$^3$. The concentration of hydrogen in the nickel at the outer surface is negligible. Determine the mass flow rate of hydrogen by diffusion through the nickel container.

**SOLUTION** Pressurized hydrogen gas is stored in a spherical container. The diffusion rate of hydrogen through the container is to be determined.

***Assumptions*** **1** Mass diffusion is *steady* and *one-dimensional* since the hydrogen concentration in the tank and thus at the inner surface of the container is practically constant, and the hydrogen concentration in the atmosphere and thus at the outer surface is practically zero. Also, there is thermal symmetry about the center. **2** There are no chemical reactions in the nickel shell that result in the generation or depletion of hydrogen.

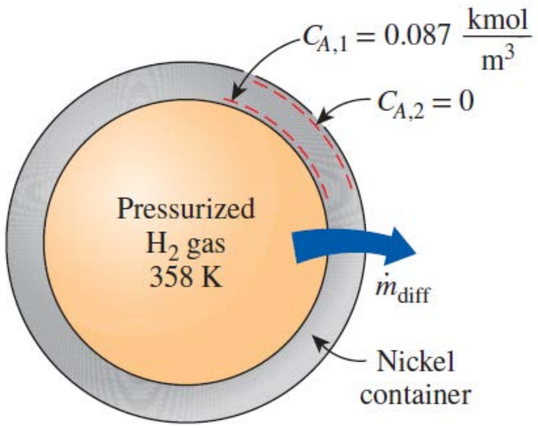



**FIGURE 14–23**
Schematic for Example 14–5.

***Properties*** The binary diffusion coefficient for hydrogen in the nickel at the specified temperature is $1.2 \times 10^{-12}$ m$^2$/s (Table 14–3*b*).

***Analysis*** We can consider the total molar concentration to be constant ($C = C_A + C_B \cong C_B =$ constant), and the container to be a *stationary* medium since there is no diffusion of nickel molecules ($\dot{N}_B = 0$) and the concentration of the hydrogen in the container is extremely low ($C_A \ll 1$). Then the molar flow rate of hydrogen through this spherical shell by diffusion can readily be determined from Eq. 14–28 to be

$$\dot{N}_{\text{diff}} = 4\pi r_1 r_2 D_{AB} \frac{C_{A,1} - C_{A,2}}{r_2 - r_1}$$

$$= 4\pi(2.34 \text{ m})(2.40 \text{ m})(1.2 \times 10^{-12} \text{ m}^2/\text{s}) \frac{(0.087 - 0) \text{ kmol/m}^3}{(2.40 - 2.34) \text{ m}}$$

$$= 1.228 \times 10^{-10} \text{ kmol/s}$$

The mass flow rate is determined by multiplying the molar flow rate by the molar mass of hydrogen, which is $M = 2$ kg/kmol,

$$\dot{m}_{\text{diff}} = M\dot{N}_{\text{diff}} = (2 \text{ kg/kmol})(1.228 \times 10^{-10} \text{ kmol/s}) = \mathbf{2.46 \times 10^{-10} \text{ kg/s}}$$

Therefore, hydrogen will leak out through the shell of the container by diffusion at a rate of $2.46 \times 10^{-10}$ kg/s or 7.8 g/year. Note that the concentration of hydrogen in the nickel at the inner surface depends on the temperature and pressure of the hydrogen in the tank and can be determined as explained in Example 14–3. Also, the assumption of zero hydrogen concentration in nickel at the outer surface is reasonable since there is only a trace amount of hydrogen in the atmosphere (0.5 part per million by mole numbers).

From Cengel