University Of Jordan
Faculty of Engineering and Technology
Department of Chemical Engineering

Transport Phenomena II

Lec 2: The Differential Equation For Mass Transfer

Content
Mass Transfer Equation

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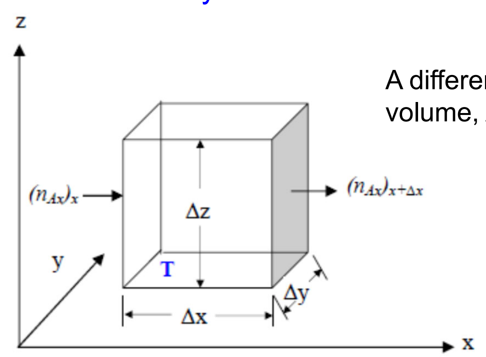
Differential Equation for Mass Transfer

- A general equation for mass transfer of a component of a binary mixture of A+B can be derived by considering all the possible changes such as molecular diffusion, bulk flow and chemical reaction at unsteady-state:



A differential control volume, Δx Δy Δz

$$\left\{\begin{array}{c}\text{net rate of mass}\\ \text{efflux of } A \text{ from}\\ \text{control volume}\end{array}\right\} + \left\{\begin{array}{c}\text{net rate of accum-}\\ \text{ulation of } A \text{ within}\\ \text{control volume}\end{array}\right\} - \left\{\begin{array}{c}\text{rate of chemical}\\ \text{production of } A\\ \text{within the control}\\ \text{volume}\end{array}\right\} = 0$$

Differential Equation for Mass Transfer

- The net rate of mass flux of constituent *A* will be

$$\text{in the } x \text{ direction:} \quad N_{A,x}\,\Delta y\,\Delta z|_{x+\Delta x} - N_{A,x}\,\Delta y \Delta z|_{x}$$

$$\text{in the } y \text{ direction:} \quad N_{A,y}\,\Delta x \Delta z|_{y+\Delta y} - N_{A,y}\,\Delta x \Delta z|_{y}$$

$$\text{in the } z \text{ direction:} \quad N_{A,z}\,\Delta x \Delta y|_{z+\Delta z} - N_{A,z}\,\Delta x\,\Delta y|_{z}$$

- The rate of accumulation of *A* in the control volume is

$$\frac{\partial C_A}{\partial t}\Delta x \Delta y \Delta z$$

- If *A* is produced within the control volume by a chemical reaction at a rate r_A, where r_A has the units (mass of *A* produced)/(volume)(time), the rate of production of *A* is

$$r_A \Delta x \Delta y \Delta z$$

Differential Equation for Mass Transfer

$$N_{A,x}\,\Delta y \Delta z|_{x+\Delta x} - N_{A,x}\,\Delta y \Delta z|_{x} + N_{A,y}\,\Delta x \Delta z|_{y+\Delta y} - N_{A,y}\,\Delta x \Delta z|_{y} + N_{A,z}\,\Delta x \Delta y|_{z+\Delta z}$$
$$- N_{A,z}\,\Delta x \Delta y|_{z} + \frac{\partial C_A}{\partial t}\Delta x \Delta y \Delta z - r_A \Delta x \Delta y \Delta z = 0$$

Dividing through by the volume Δx Δy Δz and taking the limit as Δx Δy Δz approach zero,

$$\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z} + \frac{\partial C_A}{\partial t} - r_A = 0$$

The *equation of continuity* for component *A*

- A similar equation of continuity may be developed for a second constituent *B* in the same manner. The differential equations are

$$\frac{\partial N_{B,x}}{\partial x} + \frac{\partial N_{B,y}}{\partial y} + \frac{\partial N_{B,z}}{\partial z} + \frac{\partial C_B}{\partial t} - r_B = 0$$

The *equation of continuity* for component *B*

One-Dimensional Molecular Diffusion Equation

- When the velocity of the mixture is zero and no chemical reaction takes place,

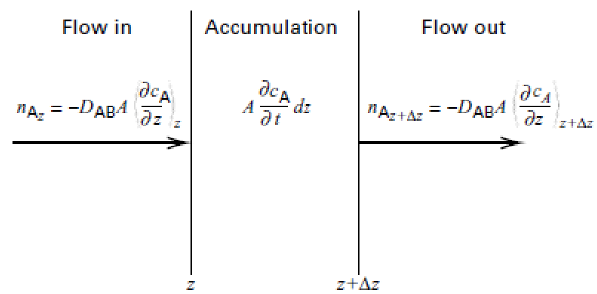
$$J_A^* = N_A = -D_{AB}\left(\frac{\partial c_A}{\partial x} + \frac{\partial c_A}{\partial y} + \frac{\partial c_A}{\partial z}\right) \quad \Rightarrow \quad \frac{\partial c_A}{\partial t} = D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2}\right)$$

Fick's second law

- For one-dimensional mass transfer of species A in stationary B through a differential control volume with no fluid motion and hence molecular diffusion in the z-direction

$$\Rightarrow \quad \frac{\partial c_A}{\partial t} = D_{AB}\frac{\partial^2 c_A}{\partial z^2}$$

1-D Fick's second law



- The assumption of no fluid motion restricts its applicability to diffusion in solids

One-Dimensional Molecular Diffusion Equation

- At steady state

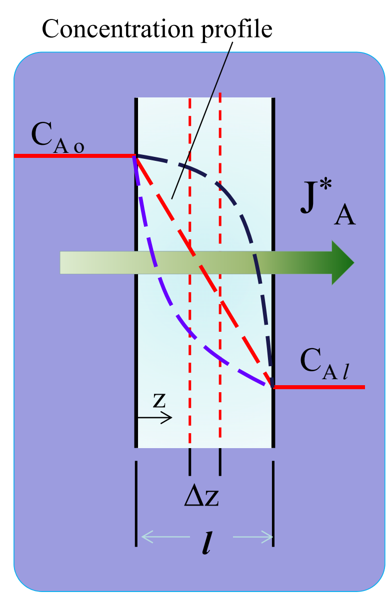
$$0 = -\frac{dJ_A^*}{dz} \quad or \quad \frac{\partial^2 c_A}{\partial z^2} = 0 \qquad \text{Constant flux over z}$$

Boundary conditions:

at z=0, $c=c_{Ao}$ at z=l, $c=c_{Al}$

$$J_A^* = -D_{AB}\frac{dc_A}{dz} \quad \Rightarrow \quad J_A^*\int_{z=0}^{l} dz = -D_{AB}\int_{c_{Ao}}^{c_{Al}} dc_A$$

$$\Rightarrow \quad \boxed{J_A^* = D_{AB}\frac{(c_{Ao} - c_{Al})}{l}}$$



b) To find the concentration profile; $c_A(z)$

$$\frac{\partial^2 c_A}{\partial z^2} = 0 \quad \overset{1^{st}\ \text{integration}}{\Rightarrow} \quad \frac{dc_A}{dz} = a$$

$$\frac{dc_A}{dz} = a \quad \overset{\text{2nd integration}}{\Rightarrow} \quad \int dc_A = a \int dz \quad \Rightarrow \quad c_A = a\,z + b$$

Using BC's

$$\Rightarrow \quad \boxed{c_A = c_{Ao} + (c_{Al} - c_{Ao})\frac{z}{l}}$$

- For cylindrical geometry

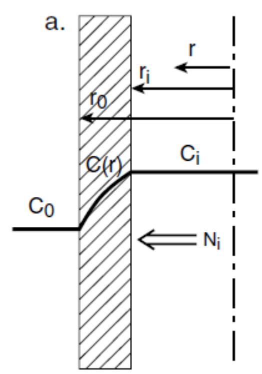
$$\frac{\partial c_A}{\partial t} = \left[\frac{1}{r}\frac{\partial}{\partial r}\left(rN_{A,r}\right) + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right] = R_A$$

- For cylindrical geometry in the r direction with no chemical reaction takes place

$$\frac{\partial c_A}{\partial t} = \frac{1}{r}\frac{\partial\left(rN_{A,r}\right)}{\partial r}$$

And with no fluid motion, i.e. $J_A^* = N_A = -D_{AB}\dfrac{dc_A}{dr}$

$$\frac{\partial c_A}{\partial t} = \frac{D_{AB}}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)$$



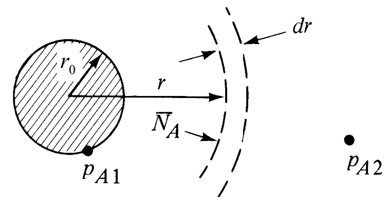
One-Dimensional Molecular Diffusion Equation

- In spherical coordinates

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

- For radial symmetry in spherical coordinates with no chemical reaction takes place

$$\frac{\partial c_A}{\partial t} = \frac{1}{r^2}\frac{\partial\left(r^2 N_{A,r}\right)}{\partial r}$$



And with no fluid motion, i.e. $J_A^* = N_A = -D_{AB}\frac{dc_A}{dr}$

$$\frac{\partial c_A}{\partial t} = \frac{D_{AB}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right)$$

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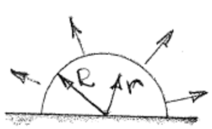
25.3 A hemispherical droplet of liquid water, lying on a flat surface, evaporates by molecular diffusion through still air surrounding the droplet. The droplet initially has a radius *R*. As the liquid water slowly evaporates, the droplet shrinks slowly with time, but the flux of the water vapor is at a nominal steady state. The temperature of the droplet and the surrounding still air are kept constant. The air contains water vapor of fixed concentration at an infinitely long distance from the droplet's surface. After drawing a picture of the physical process, select a coordinate system that will best describe this diffusion process, list at least five reasonable assumptions for the mass-transfer aspects of the water-evaporation process, and simplify the general differential equation for mass transfer in terms of the flux N_A. Finally, specify the simplified differential form of Fick's flux equation for water vapor (species *A*), and propose reasonable boundary conditions.



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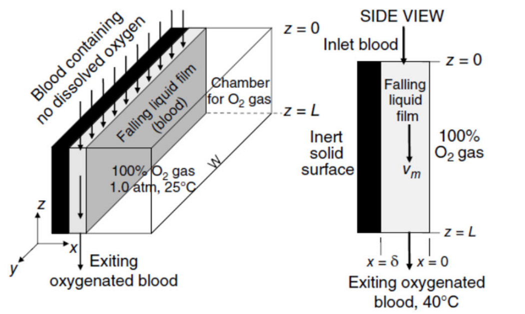
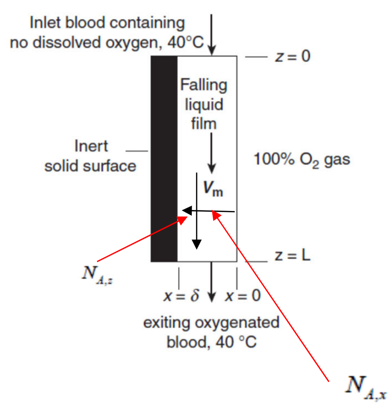
25.6 A device has been proposed that will serve as a "blood oxygenator" for a heart–lung bypass machine, as shown in the figure below. In this process, blood containing no dissolved oxygen (O_2, species A) enters the top of the chamber and then falls vertically down as a liquid film of uniform thickness, along a surface designed to appropriately wet blood. Contacting the liquid surface is a 100% O_2 gas phase. Oxygen is soluble in blood, where the equilibrium solubility c_{A^*} is function of the partial pressure of oxygen gas. In analyzing the mass transport of dissolved oxygen into the falling film, you may assume the following: (1) the process has a constant source of O_2 (gas) and a constant sink (falling liquid film), and so is at steady state; (2) the process is dilute with respect to dissolved oxygen dissolved the fluid; (3) the falling liquid film has a flat velocity profile with velocity v_{max}; *(4) the gas space always contains 100% oxygen; (5) the width of the liquid film,* W, *is much larger than the length of the liquid film,* L.

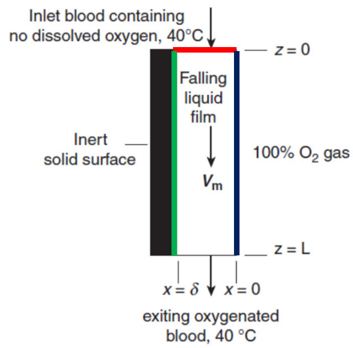
a. Simplify the general differential equation for O_2 transfer, leaving the differential equation in terms of the fluxes. If your analysis suggests more than one dimension for flux, provide a simplified flux equation for each coordinate of interest.

b. Provide one simplified differential equation in terms of the oxygen concentration c_A.

c. Provide boundary conditions associated with the oxygen mass-transfer process.







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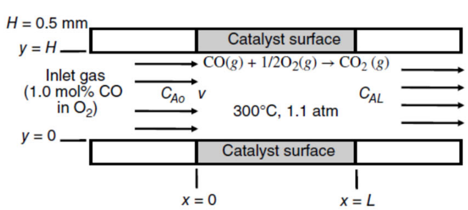
25.8 Consider the process shown in the figure below, where carbon monoxide (CO) gas is being oxidized to carbon dioxide (CO_2). This process is similar to how the catalytic converter in your car works to clean up CO in the exhaust. The inlet gas, which is 1.0 mole% CO diluted in O_2, is fed into a rectangular chamber with a nonporous catalyst layer lining the top and bottom walls. The catalyst surface drives the reaction $CO(g) + 1/2O_2(g) \rightarrow CO_2(g)$, which is extremely rapid at the temperature of operation so that the gas-phase concentration of CO at the catalyst surface is essentially zero. For this system, you may assume that the gas velocity profile is flat—i.e., $v_x(y) = \mathbf{v}$, and the gas velocity is relatively slow.

a. Develop the final form of the general differential equation for mass transfer in terms of the concentration profile for CO, c_A (species A). State all relevant assumptions, and also describe the source and sink for CO mass transfer.

b. State all necessary boundary conditions needed to specify the system.



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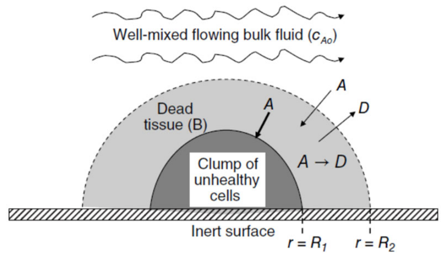
25.10 Consider the drug treatment system shown in the figure below. A hemispherical cluster of unhealthy cells is surrounded by a larger hemisphere of stagnant dead tissue (species B), which is turn surrounded by a flowing fluid. The bulk, well-mixed fluid contains a drug compound (species A) of constant but dilute bulk concentration c_{Ao}. Drug A is also soluble in the unhealthy tissue but does not preferentially partition into it relative to the fluid. The drug (species A) enters the dead tissue and targets the unhealthy cells. At the unhealthy cell boundary ($r = R_1$), the consumption of drug A is so fast that the flux of A to the unhealthy cells is diffusion limited. All metabolites of drug A produced by the unhealthy cells stay within the unhealthy cells. However, drug A can also degrade to *inert* metabolite D by a first-order reaction dependent on c_A—i.e., $A \xrightarrow{k} D$—that occurs only within the stagnant dead tissue.

a. State all reasonable assumptions and conditions that appropriately describe the system for mass transfer.

b. Develop the differential form of Fick's flux equation for drug A within the multicomponent system *without* the "dilute system" assumption. Then, simplify this equation for a dilute solution. State all additional assumptions as necessary.

c. Appropriately simplify the general differential equation for mass transfer for drug A. Specify the final differential equation in two ways: in terms of N_A, and in terms of concentration c_A.

d. Specify the boundary conditions for both components A and D.



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