

# BE.430 Tutorial: Molecular Transport/Mass Transport

9/17/2004

Chemical engineers usually have a strong background in transport phenomena and may be familiar with and have a better understanding of the concepts taught in the first few weeks of BE.430. We have therefore designed this tutorial for students who are unfamiliar with the concepts of mass transport.

Remember, however, that there are significant differences between transport occurring in chemical systems and biological systems. This tutorial summarizes only the chemical transport for background; the lectures teach you the intrigues of phenomena occurring in biological systems.

## 0. Differential Operations (more in Deen pp. 573-577)

### a. Rectangular

$$\nabla f = \frac{\partial f}{\partial x} \vec{e}_x + \frac{\partial f}{\partial y} \vec{e}_y + \frac{\partial f}{\partial z} \vec{e}_z$$

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$$

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

### b. Cylindrical

$$\nabla f = \frac{\partial f}{\partial r} \vec{e}_r + \frac{\partial f}{\partial \theta} \vec{e}_\theta + \frac{\partial f}{\partial z} \vec{e}_z$$

$$\nabla \cdot \vec{v} = \frac{1}{r} \frac{\partial}{\partial r} (r v_r) + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}$$

$$\nabla^2 f = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2}$$

### c. Spherical

$$\nabla f = \frac{\partial f}{\partial r} \vec{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \vec{e}_\theta + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \vec{e}_\phi$$

$$\nabla \cdot \vec{v} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi}$$

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}$$

## 1. Governing Equations

### a. Species conservation

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N} + R$$

b. Constitutive equation (Fick's law)

$$\vec{N} = -D \cdot \nabla c$$

c. Rate of chemical reaction

( $R$  is positive for generation, negative for consumption)

Consider a reaction  $A + B \xrightleftharpoons[k_r]{k_f} C$  and we want to find the concentration profile of  $C$ .

Then by mass conservation of  $C$ ,

$$\frac{dc_C}{dt} = k_f c_A c_B (\text{generation}) - k_r c_C (\text{consumption})$$

Generation will be dependent on concentrations of  $A$  and  $B$ , where as loss of  $C$  will be dependent on the concentration of  $C$

The change in  $c_C$  over time describes the reaction rate; therefore, at any point in the system,

$$R = k_f c_A(x) c_B(x) - k_r c_C(x)$$

Summary of most commonly encountered reaction rates:

1. *0th-order kinetics:*

$$R = k_0 [\text{conc./time}]$$

2. *1st-order kinetics*

$$R = k_1 [\text{1/time}] \cdot c(x)$$

3. *2nd-order kinetics*

$$R = k_2 [\text{1/conc.} \cdot \text{time}] \cdot c(x) \cdot a(x)$$

4. *Michaelis-Menten*

$$R = \frac{R_{\max} c(x)}{K_m + c(x)}$$

5. *and others...*

## 2. Boundary conditions

a. Constant, fixed concentrations at boundary

$$c(x_0) = c_0$$

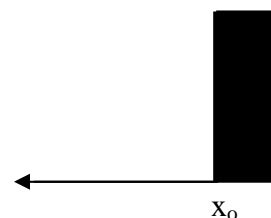


e.g. well mixed chamber separated by membrane; at membrane boundaries, we assume constant concentrations

b. No flux conditions at boundary

$$N|_{x=x_0} = -D \frac{dc}{dx} \Big|_{x=x_0} = 0$$

e.g. no flux of species at indiffusible wall



- c. Or more generally...Flux matching !

$$-D \cdot \nabla c \Big|_{x=x_0} + R = 0 \quad (\text{watch out for the signs, always consider } \vec{n}_l !)$$

e.g. reactions at the wall (heterogeneous reaction!)

NOTE: homogeneous vs. heterogeneous reactions

Homogeneous reaction: reaction occurs throughout the system

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N} + R$$

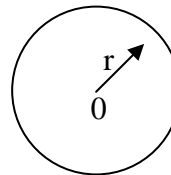
Heterogeneous reaction: reaction only occurs at system boundaries (or only at a partial volume of the system);  $R = 0$ , use flux matching to incorporate heterogeneous reaction.

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N} + R$$

- d. Geometrical symmetry

$$N \Big|_{r=0} = 0$$

e.g. at center of sphere.



### 3. Assumption/Examples for simplifications (always show in homework!)

- a. steady-state

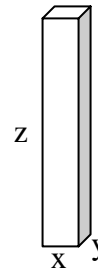
$$\text{time-independence} \left( \frac{\partial}{\partial t} \rightarrow 0 \right)$$

quasi-steady-state approximation by comparison of process time scales

- b. dimensionality

1-dimensional problem; 2-dimensional problem...

e.g. since  $z \gg x, y$ , assume conc. profile only in  $x$  and  $y$ .



- c. constant diffusivity  $D \neq f(c, x, y, z, \text{etc.})$

simplifies the governing equations in 1-D to

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + R$$

- d. no chemical reaction or heterogeneous chemical reaction

$$R = 0$$

- e. no charged species, no convection...

#### 4. Solving a mass transport problem

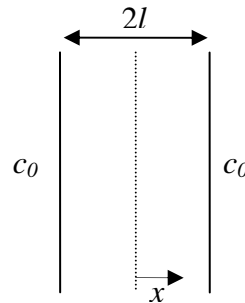
##### Example problem:

Steady-state diffusion of oxygen in slab of tissue with first-order homogeneous reaction

Consider a slab of tissue of length  $2l$  in a tank with a well-mixed solution of chemoattractant at a concentration of  $c_0$ . In the tissue, chemoattractant is consumed with first-order reaction rate  $k$ . Determine the concentration profile in the tissue.

##### a. Draw schematic of problem and label with variables

Recognize the symmetry of the problem!



##### b. State assumptions

1. steady-state
2. 1-dimensional problem (thin slab with large surface area)
3. constant diffusivity of chemoattractant
4. homogeneous first-order reaction

##### c. Set up governing equations

$$\frac{\partial c}{\partial t} = 0 = -\frac{\partial N_x}{\partial x} + R; N_x = -D \frac{\partial c}{\partial x}; R = -kc \text{ (consumption)}$$

$$\rightarrow D \frac{\partial^2 c}{\partial x^2} - kc = 0$$

##### d. Set up boundary conditions

1.  $c(x=l) = c_0$
2.  $c(x=-l) = c_0$

##### e. Solve governing equations

$$D \frac{\partial^2 c}{\partial x^2} - kc = 0 \rightarrow c(x) = Ae^{-\sqrt{\frac{k}{D}}x} + Be^{\sqrt{\frac{k}{D}}x} = C \cosh \sqrt{\frac{k}{D}}x$$

##### f. Apply boundary conditions

1.  $c_0 = C \cosh \left( \sqrt{\frac{k}{D}}l \right)$

$$2. c_0 = C \cosh\left(-\sqrt{\frac{k}{D}}l\right) = C \cosh\left(\sqrt{\frac{k}{D}}l\right)$$

$$\rightarrow C = \frac{c_0}{\cosh\left(\sqrt{\frac{k}{D}}l\right)}$$

**g. Solution**

$$c(x) = c_0 \frac{\cosh\sqrt{\frac{k}{D}}x}{\cosh\sqrt{\frac{k}{D}}l}$$

**h. Plot for conceptual understanding** (not shown here)