Homework #2 - Solutions

Released: 10/06/2014 (Mon) - Due: 10/16/2014 (Thu), 5:30 pm (Bldg 35, Room 519)

The homework will NOT be graded, but we will check for MISSING ANSWERS and CHEATING. Note that a cheated homework will get 80% of the lowest score in the class. You can give the answers <u>either</u> in English <u>or</u> Korean.

1. [Mass balance] The SNU River has a flow rate of $3.00 \text{ m}^3/\text{s}^1$. A stream named CEE discharges into the SNU River at a flow rate of $0.05 \text{ m}^3/\text{s}$. To study mixing of the stream and the river, a non-reactive compound is to be added to CEE. The detection limit for this compound is 1.0 mg/L. For the compound to be detected after the stream and the river is completely mixed and the system reaches the steady state, what is the minimum amount of the compound (in kg/day) that should be added to the stream? Assume that the compound is not present in the river and the stream prior to the addition.

¹This is a flow rate before the stream discharges to the river.

Answer) The system can be drawn as below.



The mass balance for the non-reactive compound within the control volume is:

(rate of mass accumulation) = (mass rate in) - (mass rate out)

The left hand side term is 0 when steady state is established.

 $0 = \textit{Mass rate}_{\textit{in}} - \textit{Q}_{\textit{SNU+ CEE}} \cdot \textit{C}_{\textit{SNU+ CEE}}$

 $M\!ass \; rate_{in} = \left(3.05 \; m^3/s\right) \cdot \\ \left(1.0 \; mg/L\right) \cdot \\ 10^3 \; L/m^3 \cdot \\ 10^{-6} \; kg/mg \cdot \\ 86400 \; s/day = 264 \; kg/day = 264 \; kg/da$

 [Reactors] In 1908, H. Chick reported an experiment in which he disinfected anthrax spores with 5% phenol solution. The results of his experiment are shown below. Assuming the experiment was conducted in a completely mixed batch reactor, determine the decay rate constant.

¹anthrax spore: 탄저균 포자

Time (min)	Anthrax spore concentration (numbers/mL)
0	398
30	251
60	158

Answer) For a CMBR,

 $\frac{C}{C_0} = e^{-kt} \qquad (C_0 = initial \ concentration)$

 $\ln(C/C_0) = -kt$

Calculating the values of C/C_0 at each time:

Time (min)	concentration, C	C/C_0	$\ln(C/C_0)$
0	398	1	0
30	251	0.631	-0.461
60	158	0.397	-0.924

Plotting the values of $ln(C/C_0)$ against time:



From the regression curve, we obtain $k = 0.154 \text{ min}^{-1}$.

Alternatively, you can choose the $ln(C/C_0)$ value at either 30 or 60 min to calculate the k value. For example, using the result at 60 min, $-0.924 = -k \cdot (60 \text{ min}), \ k = 0.154 \text{ min}^{-1}$

This one-point approach may be valid only for in-class problems of which data are often designed to exactly follow the first-order kinetics without any errors. In reality, the data will be somewhat scattered because of errors that can hardly be avoided (ex: measurement error). In this case, the regression approach with multiple data points should be appropriate for reliable estimation of the reaction constant.

- 3. [Reactors] A reactor with a dimension of 4 m \times 2.5 m \times 50 m (width \times depth \times length) is receiving a flow rate of 250 m³/hr. Assume that the reactor acts as an <u>ideal</u> PFR.
 - i) Calculate the retention time.

Answer) $V_{reactor} = 4 \cdot 2.5 \cdot 50 = 500 \ m^3$

$$t_0 = \frac{V_{reactor}}{Q} = \frac{500 \ m^3}{250 \ m^3/hr} = 2 \ hr$$

ii) If a terrorist dumped 10 kg of benzene to the influent, how long will it take for the benzene to be detected in the effluent (detection limit = 1 mg/L)? What will be the maximum concentration in the effluent?

Answer) Note that for a PFR, there is no mixing in the direction of flow. Therefore, the effluent benzene concentration will look like the following:



The benzene concentration will be zero for 2 hours after the terrorist dumps the benzene in the influent, then peaks to infinity at 2 hours, and then go back to zero again. Note that we are dealing with an ideal PFR.

Therefore, it takes 2 hours for benzene to be detected, and the maximum concentration goes to infinity (∞).

- 4. [Reactors] An ideal CMFR with a reactor volume of 500 m³ is receiving a flow rate of 250 m³/hr.
 - i) Calculate the retention time

Answer)
$$t_0 = \frac{V_{reactor}}{Q} = \frac{500 \ m^3}{250 \ m^3/hr} = 2 \ hr$$

ii) If a terrorist dumped 10 kg of benzene to the influent, how long will it take for the benzene to be detected in the effluent (detection limit = 1 mg/L)? What will be the maximum concentration in the effluent? How long will it take for the benzene to go below the detection limit in the effluent?

Answer) The solution for a CMFR without reaction and influent concentration is:

 $C_{out,t} = C_0 \left[\exp \left(-\frac{t}{t_0} \right) \right]$

The initial concentration, $C_0 = \frac{10 \text{ kg}}{500 \text{ m}^3} \times 10^6 \text{ mg/kg} \times 10^{-3} \text{ L/m}^3 = 20 \text{ mg/L}$

The effluent concentration will change over time as shown below:



Therefore, benzene will be detected in the effluent immediately after the benzene is dumped, and this is when the effluent benzene concentration will be at its maximum (20 mg/L).

The time for effluent benzene concentration to go below 1 mg/L is calculated by:

$$t = -t_0 \cdot \ln\left(\frac{C_{out,t}}{C_0}\right) = -\left(2 \ hr\right) \cdot \ln\left(\frac{1 \ mg/L}{20 \ mg/L}\right) = 6.0 \ hr$$

5. [Reactors] You are planning to apply chlorine disinfection to kill pathogens in a drinking water treatment plant. The pathogen decay kinetics by chlorine disinfection follows a first-order reaction with a reaction constant of 0.2/min. Your goal is to achieve 99%

reduction in the number of pathogens by the disinfection and want to determine whether you have to design a PFR or a CMFR. Assuming the flow rate is $20 \text{ m}^3/\text{min}$, calculate the volume requirement of the reactor for a PFR and a CMFR.

Answer)

i) For a PFR,

 $\frac{C_{out}}{C_{in}} = e^{-kt_0}, \ t_0 = -\frac{1}{k} \cdot \ln\left(\frac{C_{out}}{C_{in}}\right) = -\frac{1}{0.2/\min} \cdot \ln 0.01 = 23 \min$

$$V = Q \cdot t_0 = (20 \ m^3/\text{min}) \cdot (23 \ \text{min}) = 460 \ m^3$$

ii) For a CMFR,

$$\frac{C_{out}}{C_{in}} = \frac{1}{1+kt_0}, \ t_0 = \frac{1}{k} \left(\frac{C_{in}}{C_{out}} - 1 \right) = \frac{1}{0.2/\min} (100-1) = 495 \min$$

 $V = Q \cdot t_0 = (20 \ m^3/\text{min}) \cdot (495 \ \text{min}) = 9900 \ m^3$

Much more volume is required for a CMFR to obtain 99% reduction than for a PFR.

6. [Ecosystems] Explain how the atmospheric N_2 is converted to a form of nitrogen that is useful for plant growth.

Answer) A limited number of group of bacteria, such as cyanobacteria, have a capability of fixing nitrogen to ammonia, which is an available form of nitrogen for plants. The nitrogen fixation also occurs in the roots of legume family plants (e.g., beans or peanuts) by symbiosis of the plants and the microorganisms living in the root region. Humans have developed a process (Haber-Bosch) to fix the atmospheric nitrogen to ammonia, which is then made as a fertilizer and be applied to facilitate plant growth.

7. [Ecosystems] Draw the typical temperature and dissolved oxygen profile in summer for a

lake located in a region of a temperate climate. Explain what happens in late fall when the temperature above the lake goes below 4°C.

Answer)



Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

(a) Temperature profile

(b) Dissolved oxygen profile

The pale red lines represent the temperature and the DO concentration for a lake in a region of a temperate climate. At the top layer, epilimnion, relatively high and constant temperature is maintained because of heating on the surface and the mixing of the heated water into the entire layer because of the wind action. The oxygen diffuses into the water from the surface, and same logic applied to have nearly saturated DO concentration in the epilimnion. As water depth goes deeper, the wind action cannot further mix the water with the surface water, and the temperature and drops with depth. As the water density increases with decrease in temperature until 4°C, this temperature profile forms a stable layer without significant vertical mixing. This layer is called as thermocline. At thermocline, the DO is provided only by diffusion, and this results in steep decline of DO concentration with depth as well. As the temperature reaches close to $4^{\circ}C$ at the deep water, the water density no longer changes with depth, but stays at its maximum. Within this layer, hypolimnion, the vertical mixing is relatively greater than the thermocline. Because of the presence of thermocline on top of the hypolimnion, there is little DO in the hypolimnion.

In late fall when the air temperature goes below $4^{\circ}C$, the surface water cools down close to $4^{\circ}C$ such that the top water is no longer lighter than the bottom water. As this happens, the water in the whole depth begins to mix altogether, which is called as turnover or overturn.

8. [Risk] The recommended time weighted average air concentration for occupational exposure to water soluble Cr^{6+} is 0.005 mg/m³. This concentration is based on an assumption that the individual is generally healthy and is exposed for 8 hours per day, 5 days per week, 50 weeks per year, over a working lifetime (from age 18 to 65 years). Assuming a body weight of 75 kg and inhalation rate of 15.2 m³/d over the working life, what is the lifetime (75 years) CDI? What is the carcinogenic risk of the individual? You can find the slope factor for the inhalation of Cr^{6+} (Chromium (VI)) in Textbook Table 6-3.

Answer)

$$CDI = C \left[\frac{CR \cdot EFD}{BW} \right] \left(\frac{1}{AT} \right)$$

$$EFD = \frac{1}{3} \frac{day}{day} \cdot 5 \frac{days}{week} \cdot 50 \frac{weeks}{year} \cdot 47 \frac{years}{years} = 3916 \frac{days}{days}$$

$$CDI = \left(0.005 \frac{mg}{m^3} \right) \left[\frac{(5.2 \frac{m^3}{d}) \cdot 3916 \frac{days}{75 \frac{kg}{g}}}{75 \frac{kg}{g}} \right] \left(\frac{1}{75 \frac{years}{years}} \cdot 365 \frac{days}{years}} \right) = 1.45 \times 10^{-4} \frac{mg}{kg} - \frac{day}{day}$$

$$Carcinogenic risk = CDI \times SF = \left(4.96 \times 10^{-5} \frac{mg}{kg} - \frac{day}{day} \right) \cdot \left(42.0 \frac{kg}{y} - \frac{day}{mg} \right)$$

$$= 6.1 \times 10^{-3}$$

9. [Risk] Characterize the hazard index for a chronic daily exposure by the water pathway (oral) of 0.03 mg/kg-day of toluene, 0.06 mg/kg-day of barium, and 0.3 mg/kg-day of xylenes. You can find the oral reference dose (RfD) for those chemicals in Textbook Table 6-4.

Answer) The RfDs for the given compounds,

Toluene: 0.2 mg/kg-day

Barium: 0.2 mg/kg-day

Xylenes: 0.2 mg/kg-day.

$$HI = \frac{CDI}{RfD}$$

$$H\!I_{Toluene} = \frac{0.03 \ mg/kg - day}{0.2 \ mg/kg - day} = 0.15$$

$$HI_{Barium} = \frac{0.06 \ mg/kg - day}{0.2 \ mg/kg - day} = 0.3$$

 $H\!I_{\!X\!y\!lenes} = \frac{0.3 \ mg/kg - day}{0.2 \ mg/kg - day} \!= 1.5$

$$HI_{T} = HI_{Toluene} + HI_{Barium} + HI_{Xylenes} = 0.15 + 0.3 + 1.5 = 1.95$$