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Student Number:111223333

1) (20 points) A reactor is used to treat a waste constituent according that follows a first-order rate model. The decay constant is K. The reactor volume is V = 500 cubic meters. The steady flow rate of liquid through the reactor is $Q_{in} = Q_{out} = 50$ cubic meters per day. The concentration in the feed is C_{in}; a function of time. Concentration in the outlet is C_{out}; also a function of time.

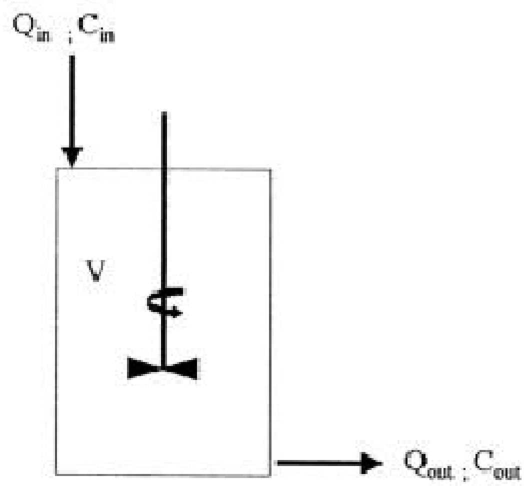

Figure 1. Reactor Sketch for Problem #1

a) Using the variables in the sketch, write the mass flow rate into the reactor.

mass_flow_in = $C_{in} * Q_{in}$

b) Using the variables in the sketch, write the mass flow rate out of the reactor.

Mass_flow_out=$C_{out}Q_{out}$

c) Assuming complete mixing, what is the concentration (using the variables above) inside the reactor?

$C = C_{out}$

d) Using the variables in the sketch, write the amount of mass accumulated within the reactor. (Calculus)

mass_acccumulated_per_time $= \frac{dCV}{dt}$

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e) Does the liquid volume in the reactor stay constant?

Yes (because we are not told Q is a function of time, we assume it is constant with respect to time). => $Q_{in} = Q_{out} = Q$

f) Write the first-order decay equation for the constituent within the reactor.

$$\frac{dC}{dt} = -KC \quad \text{or} \quad \frac{dCV}{dt} = -KVC$$

g) Using (a)-(f) write the mass balance for the constituent within the reactor.

$$\frac{dCV}{dt} = C_{in}Q - CQ - KCV$$

h) Solve the equation in (g) for steady state conditions.

$$\frac{dCV}{dt} = C_{in}Q - CQ - KCV \quad \text{the time derivative vanishes at steady state}$$

$$0 = C_{in}Q - CQ - KCV \quad \text{rearrange and isolate “C”}$$

$$CQ + KCV = C_{in}Q \quad \text{(step 1)}$$
$$C(Q + KV) = C_{in}Q \quad \text{(step 2)}$$
$$C = \frac{C_{in}Q}{(Q + KV)} \quad \text{(done!)}$$

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2) (20 points) The reactor in problem 1 was operated under the conditions above, and the following data were collected at the outlet.

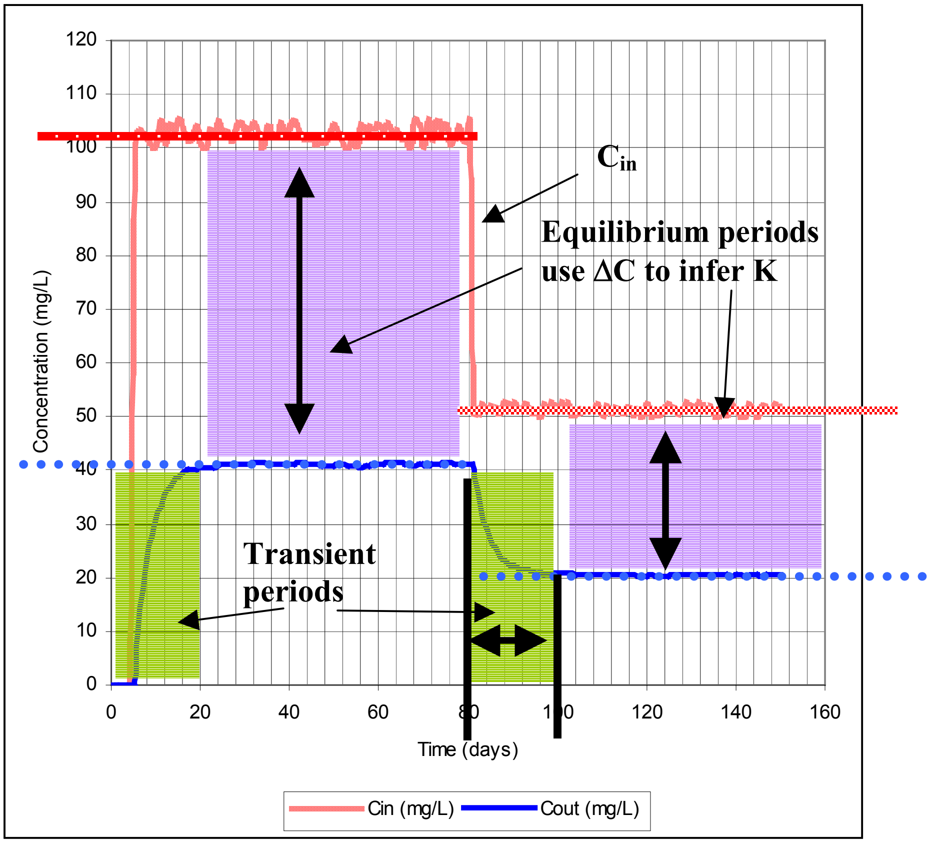

Figure 2. Data from Reactor Operation

1) Use the results of your analysis (Problem 1) and the figure above to determine the value of the decay constant in reciprocal days (day^{-1}).

Use chart to estimate Cin and C during a non-transient period of time.

$$C = \frac{C_{in}Q}{(Q+KV)} \quad \text{(start here and isolate K)}$$

$$K = \frac{C_{in}Q - CQ}{CV} \quad \text{(done!)}$$

$$K = \frac{100(50) - 40(50)}{40(500)} = 0.15 d^{-1}$$

2) Use the results of your analysis and the figure above to estimate the time for the reactor reach a new equilibrium after a change in the input concentration.

Pick a transient period, duration is about 20 days.

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3) (10 points) Hydrochloric acid, HCl, completely ionizes when dissolved in water. Calculate the pH of a solution containing 25 mg/L of HCl.

HCl <> H_{+} + CL^{-}

Complete inoization means that one mole of HCL produces one mole H^{+} and one mole Cl^{-}

Thus need to find how many moles in 25 mg

$$25mgHCL * \frac{1molHCL}{36{,}000mg} = 6.94x10^{-4} molHCL$$

$$6.94x10^{-4} molHCL \rightarrow 6.94x10^{-4} H^{+}$$
$$pH = -\log[6.94x10^{-4}] = 3.15$$

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4) (15 points) Consider the reaction representing combustion of propane in an oxygen atmosphere.

$$C_3H_8 + O_2 \Rightarrow CO_2 + H_2O$$

a) Balance the equation
b) How many moles of oxygen are required to burn one mole of propane?
c) How many grams of oxygen are required to burn 100 grams of propane?
d) At STP (1 atm, 25 ^oC) what volume of oxygen is required to burn 100g of propane?
e) At STP, air is 21% oxygen. What volume of air is required to burn 100 grams of propane?
f) At STP what volume of CO_2 is produced when 100 grams of propane are burned?

a) $C_3H_8 + 5\ O_2 \Rightarrow 3\ CO_2 + 4\ H_2O$

b) 5 mol O_2 per 1 molC_3H_8

c) $$100gC_3H_8 \frac{1molC_3H_8}{44gC_3H_8}\frac{5molO_2}{1molC_3H_8}\frac{32gO_2}{1molO_2} = 363gO_2$$

d) $$363gO_2\frac{1molO_2}{32gO_2}\frac{24.4L(@25^oC)}{1mol} = 277L - O_2$$

e) $$277L\frac{100L-air}{21L-O_2} = 1320L - air$$

f) $$100gC_3H_8\frac{1molC_3H_8}{44gC_3H_8}\frac{3molCO_2}{1molC_3H_8}\frac{44gCO_2}{1molO_2} = 314gCO_2$$

$$314gCO_2\frac{1molCO_2}{44gCO_2}\frac{24.4L(@25^oC)}{1mol} = 174L - CO_2$$

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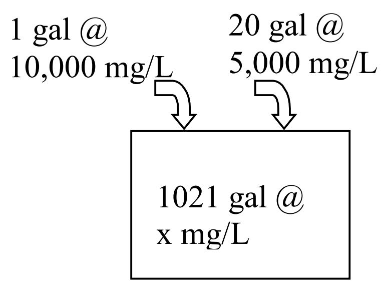
(15 points) One individual pours one gallon containing 10,000 mg/L of a hazardous chemical into 1,000 gallons of water. A second person pours 20 gallons containing 5,000 mg/L of the same chemical in the water. You learn that the chemical formula of this highly biodegradable chemical is $C_{10}H_{20}$. You collect a 5-mL sample for your laboratory to analyze. What laboratory results do you expect for:

a. Concentration of the chemical after the second individual has added their 20 gallons (express results in ppm)?
b. The COD in the 5-mL sample in mg/L?

Sketch:



g) Find total mass, divide by total volume, convert to ppm.

$$\frac{(1gal)(10000mg/L)+(20gal)(5000mg/L)}{1020gal}=107mg/L$$

This is a relatively dilute solution so C = ~ 107 ppm. (If you convert the 1L to a mass, you will arrive at nearly the same result)

h) $C_{10}H_{20} + 15\ O_2 \Rightarrow 10CO_2 + 10\ H_2O$

$$\frac{107mgC_{10}H_{20}}{L}\frac{1molC_{10}H_{20}}{140gC_{10}H_{20}}\frac{15molO_2}{1molC_{10}H_{20}}\frac{32gO_2}{1molO_2}=\frac{367mg}{L}O_2$$

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4) (20 points) Given the pH of a water-carbonate system that is closed to the atmosphere, with residual carbonate solid present, and the concentration of H_2CO_3, determine the concentration of the other species in solution.

a) First look up the relevant equilibrium constants for the equilibria below:

(1) $H_2O <> H^+ + OH^-$	$K_w = 1 \times 10^{-14}$ M
(2) $CaCO_3 <> Ca^{2+} + CO_3^{2-}$	$K_{sp} = 4.57 \times 10^{-9}$ M
(3) $H_2CO_3 <> H^+ + HCO_3^-$	$K_{a1} = 4.47 \times 10^{-7}$ M
(4) $HCO_3^- <> H^+ + CO_3^{2-}$	$K_{a2} = 4.68 \times 10^{-11}$ M

b) Write the law of mass action for the equilibria:

(1) $[H^+][OH^-] = K_w = 1 \times 10^{-14}$ M

(2) $[Ca^{2+}][CO_3^{2-}] = K_{sp} = 4.57 \times 10^{-9}$ M

(3) $\dfrac{[H^+][HCO_3^-]}{[H_2CO_3]} = K_{a1} = 4.47 \times 10^{-7}$ M

(4) $\dfrac{[H^+][CO_3^{2-}]}{HCO_3^-} = K_{a2} = 4.68 \times 10^{-11}$ M

c) Write the charge Balance:

$[H^+] + 2[Ca^{2+}] = [OH^-] + [HCO_3^-] + 2[CO_3^{2-}]$

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Finally, In a system closed to the atmosphere the following holds:

$[Ca^{2+}] = [H_2CO_3] + [HCO_3^-] + [CO_3^{2-}]$

For this problem you are given:

pH = 9.95 ; $[H^+]=10^{-9.95}$

$[H_2CO_3] = 2.5 \times 10^{-8}$

Find:

d) $[Ca^{2+}] = [4.57 \times 10^{-9}] / [4.15 \times 10^{-5}] = 1.1 \times 10^{-4}$ M

e) $[CO_3^{2-}] = [4.68 \times 10^{-11}][9.96 \times 10^{-5}] / [10^{-9.95}] = 4.15 \times 10^{-5}$ M

f) $[HCO_3^-] = [4.47 \times 10^{-7}][2.5 \times 10^{-8}]/[10^{-9.95}] = 9.96 \times 10^{-5}$ M

g) $[OH^-] = [10^{-14}]/[10^{-9.95}] = 8.9 \times 10^{-5}$ M

Verify that your results satisfy the charge balance.

$[H^+] + 2[Ca^{2+}] = 2.2 \times 10^{-4}$

$[OH^-] + [HCO_3^-] + 2[CO_3^{2-}] = 2.27 \times 10^{-4}$

Close, difference is ~ 10^{-5}. Cause is rounding error propagation and our book uses different acid-base dissociation constants than problem source.