### **Chemistry of Farming**

#### **<u>Question #1:</u>** (29 points)

A crucial component in today's agricultural industry is fertilizer. Without fertilization, farms would not be able to produce the incredible amount of food the world needs at such a high rate.

a. Fertilizers that contain nitrogen almost always contain it in the form of ammonia or one of its derivatives. Ammonia is synthesized from gaseous nitrogen and hydrogen in the following reaction:

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

i. The heat of formation of ammonium is -92 kJ/mol. With this information, explain why it can be challenging to find the optimal temperature that maximizes the rate of ammonia production. You should include both equilibrium and kinetic arguments in your answer. *(4 points)* 

Since the formation of ammonium is an exothermic process, lowering the temperature of the reaction would shift the equilibrium toward the products. However, if the temperature is too low, the rate of the reaction will be too slow. Thus, temperature must be balanced between these two factors.

+2 points for identifying that increasing temperature shifts equilibrium toward reactants OR decreasing temperature shifts equilibrium toward products
+2 points for identifying that increasing temperature increases rate OR decreasing temperature decreases rate

ii. To maximize the amount of ammonia synthesized, should high pressures or low pressures be used, and why? You should include both equilibrium and kinetic arguments in your answer. *(3 points)* 

High pressures. High pressure favors ammonia formation because the product side of the equation has fewer moles of gas. High pressure also increases the rate of the reaction because it increases the frequency/likelihood of molecular collisions.

- +1 point for saying high pressure
- +1 point for identifying that the right side of the equation has fewer moles of gas
- +1 point for identifying that high pressure increases the frequency of collisions
  - iii. The conditions that a particular manufacturer uses to produce ammonia are 450 °C and 200 atm. The reaction takes place in an industrial-sized chamber that is 100 cubic meters in volume. Assuming ideal gas behavior, how many moles of gas can the chamber contain under these conditions? Give answer in kmol. (3 points)

Using the ideal gas law, PV = nRT, where P = 200 atm, V = 100,000 L, R = 0.0821, and T is 723 K. Solving for n gives 337,000 moles of gas which is **337 kmol**.

+1 **point** for work showing substitution of values into ideal gas law PV=nRT (or a similar process)

+2 points for correct final answer 337 kmol

**Note #1:** If student does not convert to kmol but has the correct answer in moles, then the student can earn a <u>maximum</u> of **2 points**.

**Note #2:** If student does not have any work, and just a correct answer, with proper units or not, then a maximum of **1 point** can be awarded.

iv. A new chamber of an unknown volume is initially filled with 150.0 atm of H<sub>2</sub> and 50.0 atm of N<sub>2</sub> and is left alone until it reaches equilibrium (the pressure is allowed to change over time and is not maintained at 200 atm). At equilibrium, the partial pressure of NH<sub>3</sub> is 20.0 atm. Calculate K<sub>C</sub> for the reaction at 450 °C. (6 points)

This problem takes advantage of the idea that partial pressures are just mole fraction!

20 atm 
$$NH_3 : 150.0 atm H_2 - 20 atm \left(\frac{3H_2}{2NH_3}\right) = 120.0 atm H_2 @ equilibrium$$
  
20 atm  $NH_3 : 50.0 atm N_2 - 20 atm \left(\frac{1N_2}{2NH_3}\right) = 40.0 atm N_2 @ equilibrium$ 

Since we do not know the volume of this new reactor, we need to get the Kc value from the Kp value as we are unable to convert from pressures to concentrations.

$$K_{p} = \frac{\left(P_{NH_{3}}\right)^{2}}{\left(P_{H_{2}}\right)^{3} * \left(P_{N_{2}}\right)} = \frac{(20 \ atm)^{2}}{(120 \ atm)^{3} * (40 \ atm)} = 5.787 \cdot 10^{-6}$$
$$K_{p} = K_{c} (RT)^{\Delta n} \therefore K_{c} = \frac{K_{p}}{(RT)^{\Delta n}}$$
$$\Delta n = 2 - 4 = -2$$
$$K_{c} = \frac{5.787 \cdot 10^{-6}}{\left(\left(0.08206 \ \frac{L \cdot atm}{mol \cdot K}\right) (450 + 273K)\right)^{-2}} = 0.02037$$
$$K_{c} = 0.02037$$

+1 **point** for correctly calculating that the partial pressures of N2 and H2 at equilibrium conditions.

+3 points for correctly solving for Kp

+2 points for correct final answer of Kc

Alternative route: solving for Kc by calculating concentrations at equilibrium.

**Note:** Due to the length and nature of this problem, if insufficient work is provided (little to no written work and/or no indication of utilized equations) then the maximum number of points that can be awarded is **1 point**.

v. A different scientist determines that the  $K_p$  for this reaction is 4.51 x 10<sup>-5</sup> at 450 °C. Using this  $K_p$  value (not your calculated value from iv), calculate  $\Delta S^\circ$  for the forward reaction for the synthesis of two moles of ammonia with units of (J/molK). Interpret the sign of your answer and explain why your value makes sense (if you don't think you got the right value, you can explain why it doesn't make sense). (8 points)

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$
,  $K_{p, NEW} = 4.51 \cdot 10^{-5}$   
 $\Delta H^\circ = -92 \text{ kJ/mol}$   $T = 450 \text{ °C}$   $P = 200 \text{ atm}$   $V = 100 \text{ m}^3$ 

Here we need to use equilibrium data to examine thermodynamic properties, so the first equation that should be used is:

$$\Delta G^o = -RT \ln K_p$$

$$\Delta G^{o} = -\left(8.314 \frac{J}{mol \ K}\right) (723 \ K) \ln(4.51 \cdot 10^{-5}) = -22.2 \frac{kJ}{mol}$$

Now we need to find the change in entropy meaning we can use the common thermodynamics equation:

$$\Delta G^o = \Delta H^o - T \Delta S^o$$

$$\Delta S^{o} = \frac{(\Delta G^{o} - \Delta H^{o})}{-T} = \frac{\left(22.2 \frac{\text{kJ}}{\text{mol}} - \left(-92 \frac{\text{kJ}}{\text{mol}}\right)\right)}{-723 K} = -158 \frac{J}{\text{mol K}}$$

This negative sign corresponds to a **decrease** in entropy. This makes sense because 4 molecules of gas reacts to form 2 molecules of gas, **decreasing the number of particles** in the system.

+1 point for using  $\Delta G^{\circ} = -RTlnK$  equation.

+2 points for correctly calculating that  $\Delta G^\circ = -22.2$  kJ/mol or 22,200 J/mol

+1 point for substituting values into the equation  $\Delta G^{\circ} = \Delta H^{\circ} - T\Delta S^{\circ}$ 

+2 points for correct final answer of -158 J/mol·K (must have correct units to earn this point!)

<u>Note:</u> Due to the length and nature of this problem, if insufficient work is provided (little to no written work and/or no indication of utilized equations) then the maximum number of points that can be awarded for the calculation portion of this problem is **1 point.** 

Interpretation of the sign of their entropy value:

+2 points for mentioning that the <u>negative</u> sign **does make sense and** corresponds to a **decrease in entropy.** This makes sense because we are **decreasing the number of gas molecules** present which corresponds to a decrease in entropy.

#### <u>OR</u>

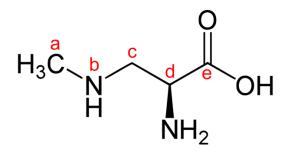
+2 points for mentioning that the <u>positive</u> sign **does make sense and** corresponds to an **increase in entropy.** This does not makes sense because we are **decreasing the number of gas molecules** present which corresponds to a decrease in entropy which is inconsistent with the result.

vi. A derivative of ammonia that is present in fertilizers is ammonium nitrate, NH<sub>4</sub>NO<sub>3</sub>. One method of synthesizing this is reacting ammonium chloride with silver nitrate. Write out the <u>net ionic</u> equation for this reaction and state the reaction type. *(2 points)* 

 $NH_4Cl + AgNO_3 \rightarrow NH_4NO_3 + AgCl$ Double replacement/displacement (also accept metathesis)

+1 point for correct chemical reaction

- +1 point for correct classification of chemical reaction
- b. For all its benefits, the industrial use of fertilizer can have some devastating consequences on the environment. The most harmful side-effect of fertilizer occurs when it is washed into neighboring waterways, causing eutrophication, a process where excessive nutrients in water lead to overgrowth of algae and cyanobacteria. This event damages biodiversity and can kill off animal life.
  - i. Cyanobacteria produce  $\beta$ -methylamino-L-alanine (BMAA), a derivative of the amino acid alanine that has neurotoxic properties, amplified to large amounts in eutrophic bodies of water. The molecule is shown below. List the letter(s) corresponding to chiral centers, or state if there are none. *(2 points)*



Answer: ONLY d

+2 point for correct answer (all or nothing). If any other locations are denoted as chiral **0** points will be awarded.

ii. Other agricultural products that can affect wildlife as run-off are pesticides, which poison fish and other organisms living in rivers. If it takes 50.0 hours for 80.0% of a certain brand of herbicide to break down in water, a first-order decomposition process, what is the rate constant for this process? Give your answer in units of inverse seconds. (3 points)

To find the half-life, use the equation:

$$(0.5)^n = 0.2 \div n = 2.322$$

This corresponds to 50 hours being equal to 2.32 half-lives. This gives the duration of a single half-life to be 21.55 hours. The rate constant for a first-order process can be solved from the half-life equation:

$$t_{1/2} = \frac{\ln 2}{k} \therefore k = 0.0322 \ hr^{-1} \left(\frac{1 \ hr}{3600 \ s}\right)$$
$$k = 8.93 \cdot 10^{-5} \ s^{-1}$$

+2 points for correctly calculating the half-life of the herbicide.

+1 **point** for correctly calculating the rate constant <u>with correct units</u>. If incorrect units are given, then this point will not be awarded!

### Problem #2: (14 points)

The driving process that underlies all forms of agriculture is photosynthesis, the process by which plants convert carbon dioxide and water into glucose represented in the formula below.

 $6CO_2 + 12H_2O + energy \rightarrow C_6H_{12}O_6 + 6O_2 + 6H_2O$ 

- a. The reaction for photosynthesis is based around the transfer of electrons a redox reaction.
  - i. Looking at the reaction equation, identify the element that is being reduced. What is its starting oxidation state, and what it its final oxidation state? *(2 points)*

Carbon is reduced and has the starting state of +4 and an ending state of 0.

+1 point saying carbon is reduced.

- +1 point saying correct starting and ending oxidation state of carbon.
- ii. Looking at the reaction equation, identify the element that is being oxidized. What is its starting oxidation state, and what it its final oxidation state? *(2 points)*

Oxygen is oxidized and has a starting state of -2 and an ending state of 0.

- +1 point saying oxygen is oxidized.
- +1 point saying correct starting and ending oxidation state of oxygen.
- iii. The energy to perform photosynthesis comes from light, and chlorophyll best absorbs blue and red light. If blue light with a wavelength of 430 nm is absorbed by chlorophyll, how much energy does the plant gain? Give final answer in Joules. (3 points)

$$E = \frac{hc}{\lambda} = \frac{\left(6.626 \cdot 10^{-34} \frac{m^2 kg}{s}\right) \left(3 \cdot 10^8 \frac{m}{s}\right)}{4.3 \cdot 10^{-7} m} = 4.62 \cdot 10^{-19} J$$

+1 point for using the energy equation above +2 point correct final answer <u>with</u> correct units!

**Note:** If student simply rights the correct answer with no work or indication of what equation they used, then **0 points** will be awarded!

iv. Assuming excess light energy, if a plant is grown in a chamber that contains 750 L of CO<sub>2</sub> gas and the plant is fed with 1L of liquid water, how many **grams** of  $C_6H_{12}O_6$  can that plant produce if it uses all the provided resources? Assume STP (0 °C and 1 atm). (7 points)

$$750 L at STP\left(\frac{1 \ mol \ CO_2}{22.4 \ L}\right) = 33.48 \ mols \ CO_2$$
$$1 L H_2O = 1000 \ mL = 1000 \ g = 55.56 \ mols \ H_2O$$

Now this has become a classic limiting reactant problem where we need to determine which reactant is limiting:

55.56 mols 
$$H_2O$$
 consumed  $\left(\frac{6 \text{ mol } CO_2 \text{ consumed}}{12 \text{ mol } H_2O \text{ consumed}}\right) = 27.78 \text{ mol } CO_2 \text{ required}$ 

<u>OR</u>

33.48 mols 
$$CO_2$$
 consumed  $\left(\frac{6 \text{ mol } CO_2 \text{ consumed}}{12 \text{ mol } H_2 0 \text{ consumed}}\right)^{-1} = 66.96 \text{ mol } H_2 0 \text{ required}$ 

Both of the calculations above imply that the water is the limiting reaction. This means that:

55.56 mols 
$$H_2O$$
 consumed  $\left(\frac{1 \text{ mol Glucose consumed}}{12 \text{ mol } H_2O \text{ consumed}}\right) = 4.63 \text{ mol glucose produced}$ 

Convert answer to grams:

$$M = 4.63 \ mol \ glucose\left(\frac{180.16 \ g \ glucose}{1 \ mol \ glucose}\right)$$

$$M = 834.1 g C_6 H_{12} O_6$$

+1 point for correctly calculating the moles of CO<sub>2</sub>

+1 point for correctly calculating the moles of H<sub>2</sub>O

+2 **point** for correctly calculating that water is the limiting reactant (with supporting work or explanation)

+3 points for correctly calculating the final mass of the glucose. If student does not give the <u>correct answer</u> in units of grams (i.e. stops at the moles of glucose), then only 1 point will be awarded.

### Problem #3: (15 points)

Current atmospheric pollution has resulted in the formation of acid rain, which is damaging to forest life and bodies of water on our planet. As acid rain becomes more potent, it can lead to major challenges with farming and agriculture.

a. The major components of acid rain are sulfuric acid, nitric acid, and carbonic acid. For each of these three acids, write balanced equations showing how gases in the atmosphere react with water to form these acids. *(3 points)* 

 $\begin{array}{l} \mathrm{SO}_3 + \mathrm{H}_2\mathrm{O} \xrightarrow{\phantom{*}} \mathrm{H}_2\mathrm{SO}_4 \\ \mathrm{NO}_2 + \mathrm{H}_2\mathrm{O} \xrightarrow{\phantom{*}} \mathrm{HNO}_3 \\ \mathrm{CO}_2 + \mathrm{H}_2\mathrm{O} \xrightarrow{\phantom{*}} \mathrm{H}_2\mathrm{CO}_3 \end{array}$ 

+1 point for each correct equation

b. Normal rain has a pH of 5.25 due to dissolved carbonic acid. If the  $K_a$  value for carbonic acid is 4.4 x 10<sup>-7</sup>, calculate the concentration of the fully protonated carbonic acid species at equilibrium in rainwater. You may ignore the second dissociation step. (4 points)

 $[H+] = [HCO3-] = 10^{-5.25} = 5.62 \times 10^{-6} M$ 4.4 x 10<sup>-7</sup> = (5.62x10<sup>-6</sup>)<sup>2</sup> / x x = **7.19 x 10<sup>-5</sup> M** 

+1 point for correct calculation of [H+]

+1 point for substituting values into correct Ka expression

+2 points for correct final answer with units.

<u>NOTE:</u> If a correct solution is written and no supporting work/indication of thought process then **0 points** will be awarded!

c. Acid rain has a pH of 4.00. Assuming that the acidity of acid rain is solely due to sulfuric acid, and assuming that both deprotonation steps of sulfuric acid proceed to completion, calculate the initial sulfuric acid concentration in acid rainwater. *(3 points)* 

 $[H^+]=10^{-pH}=10^{-4}=1.00 \times 10^{-4} M$ 

 $[H2SO4]_{initial} = 1.00 \times 10^{-4} \text{ M} / 2 = 5.0 \times 10^{-5} \text{ M}$ 

- +1 point for correct calculation of [H+]
- +2 points for correct final answer with units

<u>NOTE</u>: If a correct solution is written and no supporting work/indication of thought process then **0 points** will be awarded!

d. In **part c**, we assumed that both deprotonation steps proceeded to completion, even though the second deprotonation step of sulfuric acid has a Ka less than 1. We also assumed that carbonic acid made a negligible contribution to the acidity in the presence of sulfuric acid. Explain why we were able to make these assumptions. *(5 points)* 

We could assume that both deprotonation steps proceeded to completion because the sulfuric acid is very dilute. We could assume that carbonic acid made a negligible contribution to the acidity because **sulfuric acid is much stronger than carbonic acid**, and the H+ provided by sulfuric acid will shift the equilibrium of carbonic acid dissociation toward the left via the common ion effect, reducing the contribution of carbonic acid to the acidity.

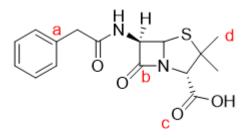
+2 points for identifying that we can assume the second deprotonation step goes to completion because the sulfuric acid is very dilute

+1 **point** for identifying that sulfuric acid is stronger than carbonic acid (or that carbonic acid is a weak acid)

+2 points for identifying that the H+ provided by sulfuric will shift the carbonic acid equilibrium to the left

### Problem #4: (19 points)

Antibiotic use in agriculture is a common and occasionally controversial topic due to their ability to combat plant and animal pathogens at the risk of conferring antibiotic resistance. In livestock feed, subclinical levels of approved antibiotics can be helpful in fighting disease and infection. Let's take a look at one potentially familiar antibiotic: benzylpenicillin.



a. Benzylpenicillin is a beta-lactam antibiotic which targets transpeptidase enzymes responsible for crosslinking peptidoglycan monomers that form the bacterial cell wall. In order to better understand the mechanism of action, a general addition-elimination mechanism is shown below.

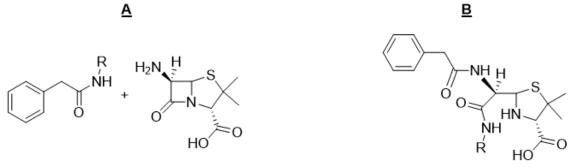
$$R-NH_2 + H_2NR \longrightarrow NH_3 + HNRRRR$$

i. Identify the hybridization of the atoms labeled A-D in the figure above. (A is carbon, B is carbon, C is oxygen, and D is carbon.) *(3 points)* 

### A, B, and C are sp2. D is sp3

+3 points for all four correct (All or nothing/No partial credit)

ii. Two possible addition elimination reactions are shown below. Select which option best represents the binding of benzylpenicillin to transpeptidase. Explain your selection. *(5 points)* 



The correct structure is B. The four-member ring is high in potential energy because its bond angles do not match the ideal 120 ° bond angles, so opening this ring is an energetically favorable process.

+1 point for identifying B
+2 point for identifying that the bond angles of the four-membered ring do not match the ideal bond angles
+2 point for identifying that the four-membered ring is high in energy OR

that the opening of the four-membered ring releases energy

#### Note: If student answers A, then 0 points will be awarded!

- b. One of the biggest concerns for antibiotic use in agriculture is the risk of conferring or accelerating the development of antibiotic resistance. While there are several mechanisms through which bacteria resist antibiotics, one of the more common ways is through mutations in the active site of a target enzyme which prevent the antibiotic from binding.
  - i. If you wanted to design a the strongest (most tightly binding) inhibitor of an enzyme's active site, would you use an inhibitor that mimics the structure of the substrate, the transition state, or the product? For the one you choose, explain why the enzyme would bind this one most tightly. (*4 points*)

Transition state. The enzyme interacts with the transition state of the reaction in order to best stabilize and lower the energy of this high energy state, thereby lowering the activation energy.

+1 point for transition state
+2 point for stating that the binding of the enzyme stabilizes / lowers the energy of the transition state

+1 point for stating that this lowers the activation energy of the reaction

ii. *Staphylococcus aureus* is one example of a Gram-positive bacterial species that may cause infections in livestock. Given that the average body temperature of a cow is approximately 38 degrees Celsius, by what factor does transpeptidase increase the rate constant of peptidoglycan crosslinking if transpeptidase lowers the activation energy by 50.2 kJ/mol? *(3 points)* 

$$\frac{k_{cat}}{k_{uncat}} = e^{\frac{50.2 \, kJ/mol}{(0.008314 \frac{kJ}{molK})(311K)}} = 2.73x10^8$$

+1 point for using the equation above +2 point for correct final answer

**Note:** If insufficient work is provided, and a correct answer is achieved, then the maximum number of points a student will be awarded is **0 points**.

Using the answer from the previous question, if a particular amount of peptidoglycan reacts in 0.0025 seconds in the presence of transpeptidase, how many days would it take for the same amount of peptidoglycan to react without a catalyst? Use your answer to briefly (in one sentence) state why enzymes are necessary for life. (4 points)

0.0025 s \* 2.73 \* 10<sup>8</sup> = 682500 s 682500 s \* 1 h / 3600 s \* 1 day / 24 h = **7.9 days** 

Enzymes are necessary because otherwise biological reactions would take way too long.

+2 points for correct final answer in days (If student had the correct final answer in units of seconds, then +1 point awarded) +2 point for correct explanation.

**<u>NOTE</u>**: Double jeopardy will not be applied. If student inputs their answer from part ii. and perform a correct calculation AND have sufficient work, then full points will be awarded.

### Problem #5: (21 points)

You are hired as a chemical consultant for a major company and are tasked with optimizing the process of the creation of a **new fertilizer** denoted Chemical X. It is proposed that this chemical is a "miracle grower" that is not carcinogenic. However, this is a very difficult chemical to produce and has only been successfully produced (at scale) under two completely different environments (temperature, pressure, reactor type, etc.). The two chemical scenarios are shown below:

Scenario #1:Overall Reaction: $A \rightarrow X \rightarrow S$	Scenario #2:Overall Reaction: $B \rightarrow X \rightarrow Q$
$A \rightarrow X$ : First order RXN	$B \rightarrow X$ : Zeroth order RXN
With rate constant $k_1$	With rate constant $k_3$
$X \rightarrow S$ : Zeroth order RXN	$X \rightarrow Q$ : First order RXN
With rate constant $k_2$	With rate constant $k_4$

As seen above the two reaction processes are series reactions where Q and S represent unwanted byproducts. A and B represent different starting reactants that Chemical X can be synthesized from.

a. In terms of the rate constants and concentrations, write the rate expressions (rate of change of concentration) for chemical species A, B, and (X in **both** scenarios) above. *(4 points)* 

$$r_A = \frac{dC_A}{dt} = -k_1 C_A$$
$$r_{X_1} = \frac{dC_{X_1}}{dt} = k_1 C_A - k_2$$
$$r_B = \frac{dC_B}{dt} = -k_3$$
$$r_{X_2} = \frac{dC_{X_2}}{dt} = k_3 - k_4 C_{X_2}$$

+1 **point** for each correct rate expression above. If the sign if off no point for that expression will be awarded! If all rate expressions match the given ones above 4 **points** will be awarded.

b. For both scenarios you want to roughly sketch out separate plots showing the concentration of each chemical over time. The initial conditions for these plots are given below.

Scenario #1 IC:  $C_A(t=0) = C_{A0}$  ,  $C_X(t=0) = C_S(t=0) = 0$ 

Scenario #2 IC:  $C_B(t=0) = C_{B0}$  ,  $C_X(t=0) = C_Q(t=0) = 0$ 

In terms of rate constants and the initial concentrations above, give the initial rates of change (slopes) of all concentrations for:

i. Scenario #1 (A, X, and S) (1 point)

Scenario #1:

$$\frac{dC_A}{dt}\Big|_{t=0} = -k_1 C_{A0}, \qquad \frac{dC_X}{dt}\Big|_{t=0} = k_1 C_{A0} - k_2, \qquad \frac{dC_S}{dt}\Big|_{t=0} = k_2$$

+1 point for having <u>ALL</u> of Scenario #1 initial slopes being correct.

ii. Scenario #2 (B, X, and Q) (1 point)

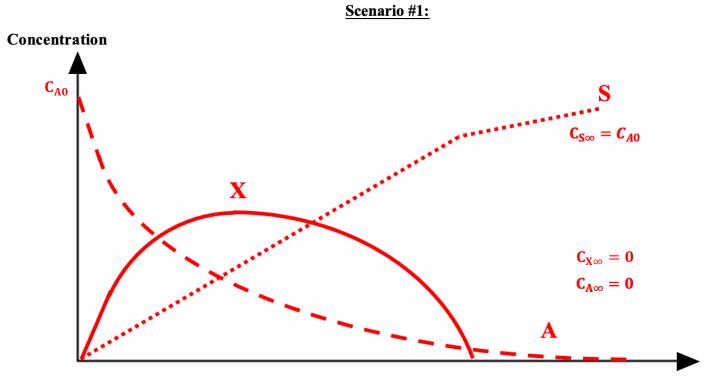
Scenario #2:

$$\frac{dC_B}{dt}\Big|_{t=0} = -k_3, \qquad \frac{dC_X}{dt}\Big|_{t=0} = k_3, \qquad \frac{dC_Q}{dt}\Big|_{t=0} = 0$$

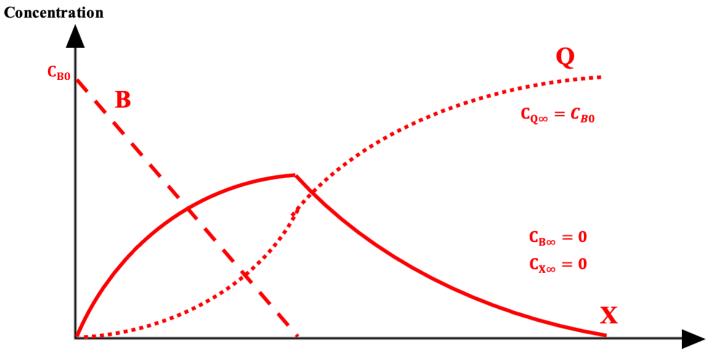
+1 point for having <u>ALL</u> of Scenario #2 initial slopes being correct.

**Note:** Because this problem is pretty much "plugging in numbers", if a student gets even one of these incorrect, then they lose the corresponding scenario's point.

c. Using the empty plots on the next page, or ones you draw yourself, sketch the concentrations of all chemicals for each scenario. Make sure to indicate the concentration of each species as time approaches infinity. Label each line <u>clearly</u>. (12 points).



time



Scenario #2:

time

#### Scenario #1 (Plot #1): (6 points total)

Plots before the concentration of X is depleted:

+1 point for plotting the concentration of A as decreasing at a decreasing rate (concave up)

+1 point for plotting the concentration of X to have an overall parabolic shape (concave down)

+1 point for plotting the concentration of S to have a linear slope

Plots after the concentration of X is depleted:

+2 points for plotting the concentration of S having a change in slope at this point with a smaller slope.

+1 point for indicating that the concentration of S approaches C<sub>A0</sub>.

#### Scenario #2 (Plot #2): (6 points total)

Plots before the concentration of B is depleted:

+1 point for plotting the concentration of B as a negative linear slope.

+1 point for plotting the concentration of X as increasing at a decreasing rate (concave down)

+1 **point** for plotting the concentration of Q as increasing at an increasing rate (concave up)

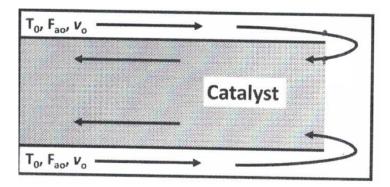
Plots after the concentration of B is depleted:

+1 point for plotting the concentration of X as decreasing at a decreasing rate (concave up)

+1 point for plotting the concentration of Q as increasing at a decreasing rate (concave down).

+1 point for indicating that the concentration of Q approaches C<sub>B0</sub>.

d. After reviewing both processes, you decide to select Scenario #1 due to overall economics. You propose the following reactor design. Liquid phase reactant A, with inlet temperature  $T_0$ , inlet molar flow  $F_{ao}$ , and volumetric flow  $v_o$ , will be fed through the annular region. Once the feed reaches the end of the annular region, it the enters the inner tube which is packed with a catalyst that will allow for both irreversible reactions (reactant A to product X and product X to unwanted product S) to occur. Note that both reactions are highly exothermic. **Explain** one advantage and one disadvantage of this reactor in comparison to a standard packed bed reactor. (3 points).



An example solution would be:

This reactor takes advantage of the heat of reaction to **preheat** the feed stream, which will lead to faster rates (smaller reactor achieves same conversion). This can also provide some heat removal for safety purposes.

A very brief list of disadvantages are:

- Might be more difficult/expensive to get this reactor as opposed to a standard reactor.
- Can be difficult to control the temperature which is a large safety issue for exothermic irreversible reactions.
- Etc.

+2 points As long as student clearly mentions one <u>reasonable</u> and <u>realistic</u> advantage.
+1 point As long as student clearly mentions one <u>reasonable</u> and <u>realistic</u> disadvantage.

**Note:** Because this problem is quite open ended, graders will use their discretion when assigning points as students might come up with reasonable advantage or disadvantage not listed above!