**CBE3223 – Kinetics and Reactor Design**
**Midterm Exam II**

**This examination is closed book, closed notes, open calculators, and you may use a one-page (front and back) equation/study sheet. Standard or graphing calculators are okay, but no smart phones, computers, or tablets are allowed except to email or chat with your instructor.**

**Please be sure to print your name, Net ID #, instructor, the subject "CBE-UY-3223", and the date on the first page of your examination solution. Please be sure to upload all of your solutions as a single electronic file (including any derivations, explanations, or calculated answers).**

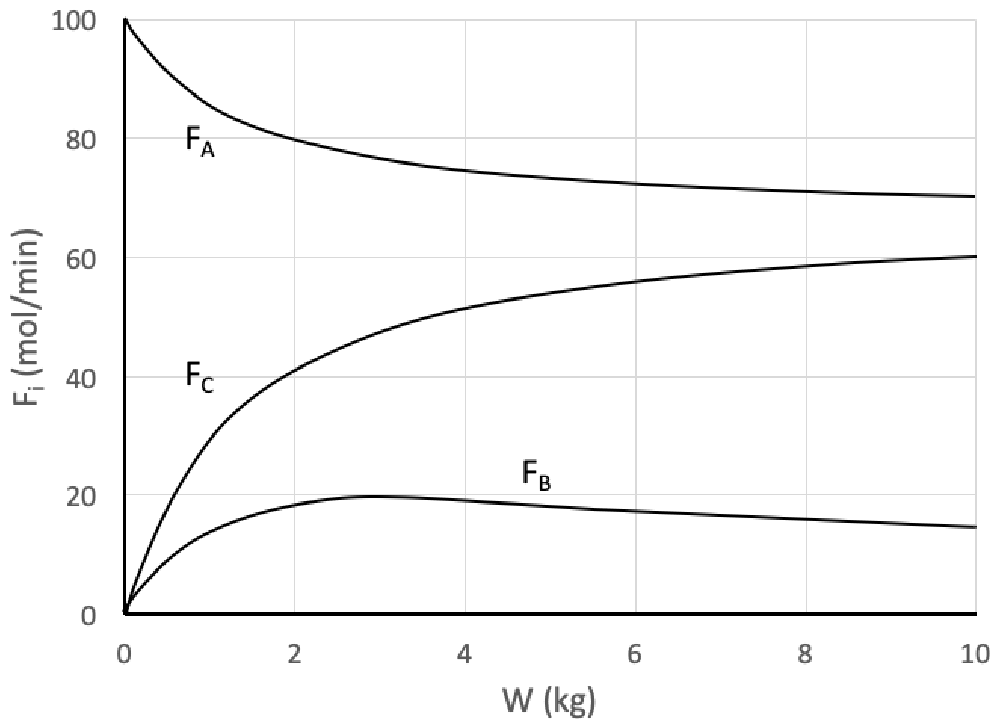
**Please note that you are expected to complete all solutions, from scratch to final draft, on your own and within 80 minutes (i.e., the normal lecture period). You are expected to follow the NYU Tandon Student Code of Conduct and NYU's Policy on Academic Integrity for Students. You are not allowed to communicate the questions or any solutions to this examination with anyone until after the completion of the 24-hour window, i.e., not until after 12:30pm ET on April 9, 2020.**

**If you have a question for clarification while taking the examination, then you may either chat with the instructor in Zoom during the in-class examination period that begins at 12:30pm ET on April 8, 2020, or you may email the instructor within the 24-hour window.**

1. An elementary dehydrogenation reaction can be represented symbolically as,

$$A \Leftrightarrow B + 2C$$

and will take place on the catalyst side of an IMRCF. The equilibrium constant for this reaction is quite small at the reaction temperature. The membrane is permeable to B, (*e.g.*, $H_2$) with a moderate mass transfer coefficient ($k_{CB}$), but not to A and C. Note that pure gaseous A is fed to the reactor. The concentration of the sweep gas is also much greater than the concentration(s) of any other species on the sweep side of the membrane. The molar flow rates of each species as a function of reactor volume are shown in the graph below.




a. **(5%)** Using dashed lines, sketch how your answer would change for a very small mass transfer coefficient for diffusion of B through the membrane. Please explain why the profiles would change (if any).

b. **(5%)** Now suppose instead that B and C diffuse through the membrane with moderate mass transfer coefficients. Using solid lines, sketch the new profiles of A, B, and C. Assume the mass transfer coefficients of B and C are the same, $k_{CC} = k_{CB}$. Please explain why the profiles would change (if any).

c. **(5%)** Suppose now a small amount of reactant A can diffuse through the membrane along with a moderate amount of B but not C. In this case, $k_{CB} > k_{CA}$. Would you expect a higher conversion in this membrane reactor compared to a packed-bed reactor with no pressure drop or membrane? Please explain your answer.

2. For the complex reactions,

$$A + B \rightarrow D \qquad -r_{1A} = k_{1A} C_A C_B^2 = \left(0.1 \frac{dm^6}{mol^2 * s}\right) C_A C_B^2$$

$$A + B \rightarrow U_1 \qquad -r_{2B} = k_{2B} C_A^2 C_B = \left(0.3 \frac{dm^6}{mol^2 * s}\right) C_A^2 C_B$$

$$B + D \rightarrow U_2 \qquad -r_{3B} = k_{3B} C_B = (0.00001\ s^{-1}) C_B$$

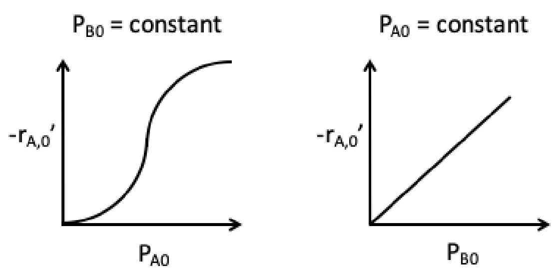
   a. **(7.5%)** Write an expression for the instantaneous selectivity, $S_{D/U}$.

   b. **(7.5%)** How, and under what conditions (e.g., reactor type(s) and concentrations), should the reactions be carried out to maximize the selectivity $S_{D/U}$?

3. **(15%)** Consider the catalytic reaction as a function of the initial partial pressures,

$$A + B \rightarrow C$$

The rate of disappearance of species A was obtained in a differential reactor and the data shown below. Propose a rate law that matches the data, and please be sure to justify your answer.




4. Consider the following enzymatic reactions,

$$E + S \overset{K_S}{\leftrightarrow} E * S$$
$$E * S + S \overset{K_S}{\leftrightarrow} S * E * S$$
$$S * E * S \overset{K_P}{\leftrightarrow} S * E * P$$
$$S * E * P \overset{k}{\rightarrow} E * S + P$$

   a. **(10%)** Derive the rate of product formation, $r_P$, for the enzymatic reactions shown above. Write your answer in terms of the equilibrium constants ($K_S$, $K_P$), specific reaction rate (k), the total enzyme concentration ($E_T$), and the substrate concentration (S).

b. **(5%)** Sketch the rate of product formation ($r_P$) as a function of the substrate ($C_S$) when substrate binding to the enzyme (E) and the enzyme substrate complex (E*S) are irreversible, which may be the case for very low substrate concentrations.

c. **(5%)** Given that $V_{max}$ = 9.09x$10^{-3}$ mol/dm$^3$/min, k = 1.0 min$^{-1}$, and $C_{Et}$ = 0.01 mol/dm$^3$ then find $K_P$.

5. Suppose the company you work with uses a 10 dm$^3$ chemo-stat to manufacture proteins for a new vaccine, and the production rate follows the Monod growth law,

$$r_g = \mu C_C = \frac{\mu_{max} C_S C_C}{K_S + C_S}$$

Assume steady-state operation and that maintenance can be neglected. Cell death, however, should not be neglected. Be sure to show all your work.

a. **(10%)** What is the dilution rate at which wash-out occurs?

b. **(5%)** Now assume that cell death can be neglected. Determine the residence time ($\tau$) and the volumetric flow rate ($\upsilon_0$) at which the cell production rate is at maximum.

c. **(5%)** Suppose the cell concentration at the dilution rate that gives the maximum production rate is 6.23 g/dm$^3$. Determine the rate of disappearance of the substrate ($-r_S$) at the maximum cell production rate. You may neglect cell death.

*Additional information:*
$\mu_{max}$ = 0.7 h$^{-1}$
$K_S$ = 0.3 g/dm$^3$
$k_d$ = 0.09 h$^{-1}$
$C_{S0}$ = 12 g/dm$^3$
$Y_{C/S}$ = 0.6 g/g

6. **(15%)** Please indicate whether each of the following statements is true ("T") or false ("F"). Please write the correct answer on your answer sheet.

T F Consider two elementary reactions in parallel where reactants A and B can form either desired (D) or undesired (U) product. If $E_D > E_U$, then the specific reaction rate for product D increases much more rapidly with temperature. Thus, the reactions should be carried out at the highest possible temperature.

T F It may not be possible to separate out the amount of substrate consumed to produce more cells from that consumed to produce product. Under these circumstances, all the substrate consumed for growth and for product formation is lumped into a single stoichiometric yield coefficient written as $Y'_{S/C}$.

T F Consider an elementary reversible reaction $A \leftrightarrow 2B + C$ carried out in a membrane reactor in which B diffuses through the membrane. Decreasing the sweep gas mass flow rate on the membrane side could result in a higher conversion for the same reactor temperature, feed conditions, and reactor volume.

T F For all types of enzyme inhibition cases we studied in lecture the rate of disappearance of the substrate (-rs) decreases with increasing inhibitor concentration (I).

T F To make the selectivity $S_{D/U} = \frac{r_D}{r_U} \approx \frac{1}{C_A^2 + C_A + 1}$ as large as possible, the reaction could be carried out in a semi-batch reactor.

T F Catalyzing a reaction with an enzyme at too high of a temperature could alter the enzyme's molecular structure and hence decrease its turnover number ($k_{cat}$) and decrease the maximum rate of reaction ($V_{max}$).

7. **(4%) Extra credit:** Recall the different phases of cell division covered during lecture. Circle the correct statement(s):

   a. In the G1 phase the cells increase in size and RNA and protein synthesis occurs.

   b. In the G2 phase RNA, protein, and DNA synthesis occurs.

   c. In the M phases the nuclear region divides and cell division occurs to give two new cells.

   d. All of the above.

*Relationships:*

For a Chemostat @ steady-state (neglecting maintenance):

$$DC_C = r_g - r_d$$

$$D(C_{S0} - C_S) = -r_S$$

Neglecting maintenance and cell death:

$$D_{maxprod} = \mu_{max}\left(1 - \sqrt{\frac{K_S}{K_S + C_{S0}}}\right)$$