CBE3223 – Kinetics and Reactor Design
Midterm Exam I
Closed book, closed notes, and open calculators
(Standard or graphing calculators are okay, but no smart phones or tablets allowed)

Please be sure to print your name, Net ID #, instructor, the subject "CBE-UY-3223", and the date on the cover of the blue book provided. Please write all answers in the bluebook (including any derivations, explanations, or solutions).

1. **(15%)** Ammonia is synthesized in the Haber Bosch process,

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \Leftrightarrow NH_3$$

which accounts for ~1.4% global carbon dioxide emissions and consumes ~1% of the world's energy. This elementary gas-phase reversible reaction is carried out in an isothermal flow reactor. The molar feed is 50% H_2 and 50% N_2, at a constant pressure of 15 atm and at a temperature of 227°C. Choosing H_2 as the basis for your calculation, write its rate law, $-r_A$, solely as a function of X, k_A ($dm^3/mol/s$), and K_C (dm^3/mol).

2. **(20%)** The following elementary reversible gas-phase reaction,

$$A \Leftrightarrow 2B$$

is carried out in a batch reactor at a constant temperature of 550 K and pressure of 10 atm. Assume that the reactor is initially charged with species A. Calculate the equilibrium conversion (X_{eb}) provided that $K_c = 1.0$ mol/dm^3.

3. **(15%)** The following irreversible elementary liquid-phase reaction,

$$A \rightarrow B + C$$

is carried out in an isothermal plug flow reactor (PFR). What Damköhler number (Da_1) is necessary to achieve conversion X = 0.79?

4. The following elementary irreversible gas phase reaction,

$$A + B \rightarrow 2C$$

is carried out in an isothermal packed-bed reactor (PBR) with pressure drop. The feed is stoichiometric in species A and B, and the entering pressure is 7 atm.

Additional information:
F_{A0} = 100 mol/min
Specific reaction rate, k_A = 0.5 mol/(atm^2*kg-cat*min)
Pressure drop parameter, α = 0.037 kg^{-1}

a. **(2.5%)** Write the mole balance in terms of conversion.

b. **(5%)** Write the rate law, $-r_A$', solely as a function of P_{A0}, X, k_A, and the catalyst mass W.

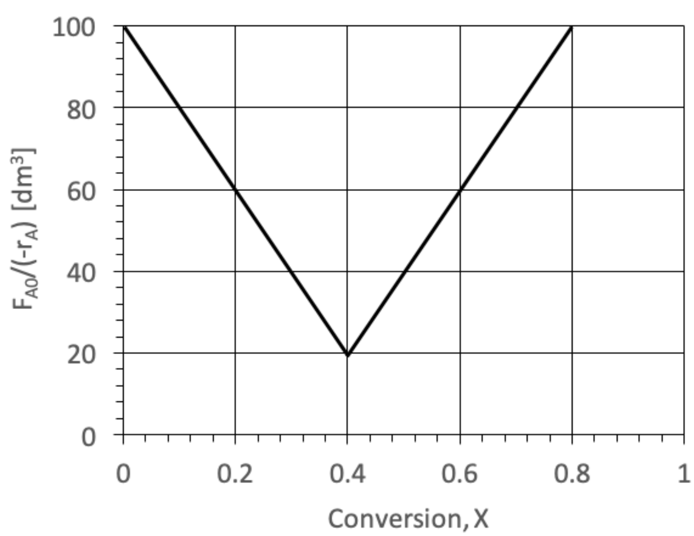
c. **(5%)** Above catalyst mass would the exit pressure fall below 3.0 atm?

d. **(7.5%)** What is the conversion exiting this PBR?

5. An adiabatic exothermic irreversible gas-phase reaction,

$$2A + B \rightarrow 2C$$

is to be carried out in a flow reactor for an equimolar feed of A and B. The Levenspiel plot for this reaction is shown below.



a. **(5%)** What PFR volume is necessary to achieve 40% conversion?

b. **(2.5%)** What CSTR volume is necessary to achieve 40% conversion?

c. **(2.5%)** What is the volume of a second CSTR added in series to the first PFR (**Part a**) necessary to achieve an overall conversion of 80%?

d. **(5%)** What PFR volume must be added to the first CSTR (**Part b**) to raise the conversion to 80%?

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

T	F	For two CSTRs in series, the overall conversion will always be greater than that of a single CSTR for isothermal reactions with power-law rate laws and reactions orders greater than zero.
T	F	The activation energy and frequency factor can be calculated if one knows the specific reaction rate at two temperatures.
T	F	By neglecting the pressure drop in a PBR, one could underestimate the reactant concentration(s) and hence overestimate their rate of disappearance and the conversion.
T	F	For isothermal operation with $\delta = 0$ and laminar flow, decreasing the particle size by a factor of 4 would increase the pressure drop parameter α by a factor of 2 and hence increase the pressure drop for the same amount of catalyst in a PBR.
T	F	For isothermal reactions greater than zero order, the rate is higher at the entrance of a PFR and gradually decreases, thereby requiring less volume (than a CSTR to achieve the same conversion) because the volume is inversely proportional to the rate.
T	F	According to collision theory, the fraction of molecular collisions that have sufficient energy to react increases with decreasing temperature.

7. **(4%) Extra credit:** For a reaction to occur, the reactants must overcome an energy barrier or activation energy E_A. The energy to overcome their barrier comes from the transfer of the kinetic energy from molecular collisions to internal energy (e.g., Vibrational Energy). Circle the correct statement(s):

   a. The molecules need energy to disort or stretch their bonds in order to break them and thus form new bonds.

   b. Factors other than concentration that affect the reaction rate include the height of the potential energy barrier, i.e., E_A, and the partial pressure.

   c. As the reacting molecules come close together they must overcome both stearic and electron repulsion forces in order to react.

   d. All of the above.

Relationships:

For a PFR: $\frac{F_A}{dV} = r_A$

And, $V = F_{A0} \int_0^X \frac{dX}{-r_A}$

For a PBR: $\frac{F_A}{dW} = r_A'$

For a CSTR: $V = \frac{F_{A0} - F_A}{-r_A}$

$$\int_0^X \frac{dX}{1-X} = ln \frac{1}{1-X}$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$\int_0^W (1 - \alpha W)\, dW = W - \frac{1}{2}\alpha W^2$$

$$\frac{dp}{dW} = -\frac{\alpha}{2p}(1 + \varepsilon X)\frac{T}{T_0}$$

Gas constant, $R = 0.082 \frac{dm^3 * atm}{mol * K}$