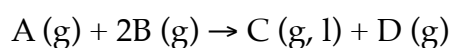


**Chemical Reaction Engineering—Homework #3**Due: Online submission on Canvas, [Wednesday, February 5, 2020 at 11:59pm.](#)

No late submissions will be accepted.

*Problems that require a numeric answer should have 3 significant figures.**Units, where required, are shown in blue. Please use these units.***Problem 1: Condensation of product in reactor**

MN Chemicals desires to run the following gas phase reaction in an isothermal, isobaric (25 deg C, 101 kPa) reactor:

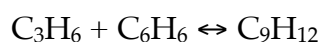


It is determined that the rate law can be expressed as first order in both reactants. The saturation mole fraction of C in the gas phase is 0.25. Assume that A and B are fed at a stoichiometric ratio and the total volumetric flow rate is 1.5 L/min. The rate constant is 0.035 L/(mol\*s). Assume that all gaseous species behave as ideal gases.

- Is this an elementary reaction/step?
- Write out the stoichiometric table in terms of  $X_A$  and  $F_{A0}$  for all species.
- What is the vapor pressure of C? At what conversion of A does condensation of C begin? [\[25 kPa, 0.6\]](#)
- Write  $(-r_A)$  both before and after condensation as a function of conversion, the rate constant, and the initial concentration of A.
- What volume of CSTR is required if you desire a conversion of 90% of A? [\[670L\]](#)

**Problem 2: Production of cumene**

You are going to produce cumene from propylene and benzene using the elementary, reversible gas phase reaction:



which as forward and reverse rate constants of  $k_f$  and  $k_r$ , respectively. The research scientists at MN Chemicals have collected the following kinetic and equilibrium data for this reaction.

| T(deg C) | $k_f$ (mol min <sup>-1</sup> L <sup>-1</sup> atm <sup>-2</sup> ) | $K_{eq}$ (atm <sup>-1</sup> ) |
|----------|--|-------------------------------|
|----------|--|-------------------------------|

|     |                  |                  |
|-----|------------------|------------------|
| 30  | $1.75 (10^{-7})$ | $9.09 (10^2)$    |
| 80  | $9.01 (10^{-5})$ | 26.3             |
| 130 | $9.83 (10^{-3})$ | 1.83             |
| 180 | $3.81 (10^{-1})$ | $2.30 (10^{-1})$ |
| 230 | 7.13             | $4.36 (10^{-2})$ |

- a. What is the activation energy and pre-exponential factor for the forward rate constant? What is the heat of reaction? [ $A = 2(10^{12})$ ,  $E_A = 110 \text{ kJ/mol}$ ,  $H_{\text{rxn}} = -63 \text{ kJ/mol}$ ]

You are synthesizing cumene using a PFR with a volume of 150L. The reactants are fed into the isothermal, isobaric reactor with a molar flow rate of 14.4 mol/min at a propylene: benzene molar ratio of 2:1 and a total volumetric flow rate of 100 L/min. Hint: Use the partial pressures of the gases instead of the molar concentrations in your rate expressions.

- b. What conversion do you achieve if the reactor is operated at 100°C? [0.1]  
 c. What conversion do you achieve if the reactor is operated at 150°C? [0.68]  
 d. Determine the equilibrium conversions at 100°C and 150°C as a function of concentrations of various species? [at 100°C,  $X = 0.95$ ; at 150°C,  $X = 0.68$ ]

### Problem 3: Gas phase batch reactor

A second order gas phase reaction,  $A \rightarrow 3B$  occurs in an isothermal batch reactor. The volume of the reactor is 10L. Initially the reactor has 50 mol of gas with 50%A and 50% inert gas. The rate constant is  $0.45 \text{ s}^{-1} \text{ M}^{-1}$ . Assume ideal gas behavior in the reactor. Calculate the conversion for this reaction after 1 minute if the reactor is operated isobarically. [0.97]

### Problem 4: Equilibrium conversions

The reversible reaction  $2A \leftrightarrow B$  is carried out in a flow reactor where pure A is fed at a concentration of 4 mol/L. The equilibrium conversion is found to be 60%. Assume that the reactor is isothermal and isobaric.

- a. What is the equilibrium constant,  $K_C$ , if the reaction is a gas phase reaction? [0.33]  
 b. What is  $K_C$  if it is a liquid phase reaction? [0.47]

The gas phase reaction  $A \leftrightarrow 3C$  is carried out in a flow reactor with no pressure drop. Pure A enters at a temperature of 400K and a pressure of 10 atm. At this temperature,  $K_C = 0.25 \text{ M}^2$ .

- c. What is the equilibrium conversion if the reaction is carried out in a constant volume batch reactor? Assume isothermal operation. [0.4]
- d. What is the equilibrium conversion if the reaction is carried out in a constant pressure batch reactor? Assume isothermal operation. [0.6]