

Introduction to Reactor Design, 3K4

Written midterm, 13 February 2013

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Note:

- You may bring in any printed materials to the midterm; any textbooks, any papers, *etc.*
- You may use any calculator during the midterm.
- You may answer the questions in any order on all pages of the answer booklet.
- *Time saving tip:* please **use bullet points** to answer, where appropriate, and **never repeat the question** back in your answer.
- Please note, parts of this exam will require you to apply concepts you have learned in your other core courses, such as 2D, 2F and 3E.
- Use the problem solving strategy we discussed in class: Define, Explore, Plan, Do It, Check, Generalize.
- Also, apply the strategy where you work symbolically, and only substitute in values at the end.
- **Total marks:** 60 marks.
- Total time: 2 hours. There are 3 pages on the exam, please ensure your copy is complete.

Question 1 [10 = 2 + 2 + 2 + 2 + 2]

Provide single word, or single short sentence answers to each of the following (no lengthy explanations, preferably no equations).

1. Give an example of a chemical reaction which has $\delta > 0$, where δ is the scalar value that measures by how much the system expands or contracts. Be sure to also supply the value of δ for your example.
2. Which of the following assumptions are required to derive the plug-flow design equation $V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$ from the general mol balance [just write the letter numbers down in your answer book]:
 - (a) the system operates at steady state
 - (b) the rate of reaction must be constant
 - (c) the reactor is well-mixed in the axial direction
 - (d) there must be no pressure drop in the axial direction
 - (e) the concentration of A in the centre-line of the reactor is the same as at the wall (also implies there is no boundary layer)
 - (f) the reactor must have the same diameter all the way from start to end to maintain constant volumetric flow

3. A first order reaction, $-r_A = k_A C_A$ is taking place in a batch reactor. If:
- $k_A = 2 \times 10^{-4} \text{ hour}^{-1}$, the reaction can be considered to be _____ (rate / equilibrium) limited.
 - $k_A = 2 \times 10^{+4} \text{ hour}^{-1}$, the reaction can be considered to be _____ (rate / equilibrium) limited.
4. In general, a liquid-phase CSTR operated at higher flow rates in and out will have _____ (lower / higher) conversion of the reagent, and will have a _____ (longer / shorter) residence time of material in the reactor.
5. If 3 CSTRs are placed in series, and a second order reaction takes place, with the requirement that each CSTR has the same amount of incremental conversion (e.g. 20% conversion per reactor), then the **last reactor** will be _____ (larger / smaller) in volume than the first reactor, and will have _____ (greater / smaller) reaction rate than the first reactor.

Question 2 [5]

The general mol balance (In - Out + Generation = Accumulation) over a boundary can be written symbolically as:

$$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt}$$

Start from this *differential* equation and end up showing that the performance equation for a CSTR is the *algebraic* equation:

$$V = \frac{F_{j0} - F_j}{-r_j}$$

Of most importance in your answer is to *show exactly how each assumption applies* in the logical progression from the starting equation to this final equation.

Question 3 [3]

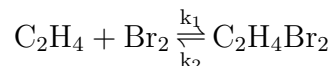
Describe why the constants in a rate expression, for example, the k_A and α constants in the expression $-r_A = k_A C_A^\alpha$, can be most conveniently evaluated in a batch reactor. *Use bullet points!* (no need to show how to calculate k_A and α).

Question 4 [12]

For the liquid phase reaction $A \rightarrow D$, with second-order kinetics and $C_{A0} = 1 \text{ mol.L}^{-1}$, we get 35% conversion after 1 hour in a batch reactor. What is the conversion and concentration of A after 1 hour if our raw material has a concentration of 5 mol.L^{-1} instead? Explain why your answer makes sense.

Question 5 [8]

At 600 K the gas-phase reaction

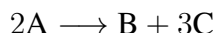


follows elementary kinetics with rate constants $k_1 = 500 \text{ L}\cdot\text{mol}^{-1}\cdot\text{hour}^{-1}$ and $k_2 = 0.032 \text{ hour}^{-1}$.

Determine an equation whose solution would yield the equilibrium conversion in a constant volume batch reactor. **Note**, the equation should contain conversion as an unknown variable. Equimolar amounts of C_2H_4 and Br_2 may be assumed to be present initially. Use appropriate symbols for any quantities that cannot be determined from the given information; numerical values for all other quantities should be inserted.

Question 6 [22]

The following gas phase reaction take place in a packed-bed reactor under isothermal conditions:



where $-r'_A = kC_A^2$ and $k = 0.6 \text{ L}^2\cdot\text{mol}^{-1}\cdot\text{min}^{-1}(\text{g catalyst})^{-1}$. The reactor operates at a temperature of 400K. The reactor is fed with an equimolar amount of A and an inert gas, I, at an inlet volumetric flow rate of $q_0 = 10 \text{ L}\cdot\text{minute}^{-1}$. The inlet pressure is 200 kPa, and the gas density at these inlet conditions is $7 \text{ kg}\cdot\text{m}^{-3}$, with viscosity of $3 \times 10^{-5} \text{ Pa}\cdot\text{s}$.

Additional information that is already known to you is that the reaction will be in a pipe of inside diameter of 5cm and length of 120 m. The catalyst can be packed leaving a void fraction of 0.5; the catalyst pellets are supplied as spheres with diameter of 0.5 cm (the volume of a sphere is $\frac{4}{3}\pi r^3$);

and the density of the catalyst is $2000 \frac{\text{kg}}{\text{m}^3 \text{ of pellet}}$.

Show all steps necessary that result in the set of 2 differential equations that can be solved, using computer software. The equations must be specified as the right hand side of:

$$\begin{aligned}\frac{dX}{dW} &= \dots \\ \frac{dy}{dW} &= \dots \\ X(W=0) &= \dots \\ y(W=0) &= \dots\end{aligned}$$

The equations should be integrated from zero to $W = \text{_____ kg}$

where X is the conversion of species A, $y = \frac{P}{P_0}$ and the catalyst weight is W .

All constants in your expressions should be evaluated and given *numerically*. Only the variables X , y and W should remain in your ODEs.

The end.