NAME: ____________________

Instructions: The exam is closed book and closed notes. Write all answers on separate paper. Do not write any answers on the exam itself. Hand in your exam as well as your solution at the end. Make sure your name is on your solution and your exam.

Exercise 1. Gas-phase reaction in a PFR. 35 points.

I told you in class that I was required by law to ask an exam question of this type, so here goes.

The following elementary, gas-phase reaction takes place in a PFR.

$$2\text{A} \longrightarrow \text{B}$$

The reactor is fed with a mixture of of reactant A and inert diluent I at feedrates N_{Af} and N_{If} at total molar concentration c_f. The feed conditions and rate constant are

$$c_f = 0.2\,\text{mol/L} \qquad N_{Af} = 2.0\,\text{mol/min} \qquad N_{If}/N_{Af} = 3 \qquad k = 20.0\,\text{L/mol}\cdot\text{min}$$

The pressure and temperature are constant in the PFR, and the gas may be assumed to behave as an ideal-gas mixture.

(a) Write a balance for the steady-state molar flow of A, N_A. Make sure that your right-hand side is a function of only N_A and known parameters. What is the initial condition for this differential equation?

(b) What reactor size is required to achieve 85 percent conversion?

(c) What happens to this reactor size if you

1. Double the rate constant k?
2. Double the feed flows N_{Af} and N_{If}, but keep feed concentration constant?
3. Double the feed concentration, but keep the feed flows constant?

Exercise 2. PFR and CSTR sizing. 35 points.

Even for a simple stoichiometry like

$$\text{A} \longrightarrow \text{B}$$

depending on the mechanism, we derived a reaction rate expression in Chapter 5 as complex as

$$r = \frac{kc_A}{(1 + Kc_A)^2}$$

(a) What are the units of k and K? Draw a sketch of $r(c_A)$ as a function of c_A. Show what happens at both low c_A concentration and high c_A concentration.

(b) Draw a sketch of $1/r(c_A)$ as a function of c_A. Find the minimum of $1/r(c_A)$. Draw this point also on your sketch.

(c) Assume we run this reaction in liquid phase in a CSTR and also in a PFR.

To achieve a conversion of A of 50 percent, and with the following parameter values, which reactor has more volume, the CSTR or the PFR?

$$c_{Af} = 1.4\,\text{mol/L} \qquad K = 2.0\,\text{L/mol}$$

Justify your answer. You might find your sketch of $1/r(c_A)$ in the previous part useful.

(d) To achieve the same 50 percent conversion of A and with the following parameter values, which reactor has more volume, the CSTR or the PFR?

$$c_{Af} = 0.6\,\text{mol/L} \qquad K = 1.0\,\text{L/mol}$$

Justify your answer. You might find your sketch of $1/r(c_A)$ in the previous part useful.

Exercise 3. Rate expression from mechanism. 30 points.

A proposed mechanism for catalytic CO oxidation

$$2\text{CO} + \text{O}_2 \longrightarrow 2\text{CO}_2$$

consists of the following steps: associative adsorption of CO, dissociative adsorption of O_2, and the bimolecular surface reaction

$$\text{CO} + \text{S} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \text{CO}_{\text{ads}}$$

$$\text{O}_2 + 2\text{S} \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2\text{O}_{\text{ads}}$$

$$\text{CO}_{\text{ads}} + \text{O}_{\text{ads}} \xrightarrow{k_3} \text{CO}_2 + 2\text{S}$$

Assume the O_2 and CO adsorption steps are at equilibrium and the surface reaction step is slow and irreversible.

(a) Find the surface concentrations $\bar{c}_{\text{CO}}$ and $\bar{c}_{\text{O}}$ as a function of the gas-phase concentrations.

(b) Given these surface concentrations find the production rate of CO_2 in terms of gas-phase concentrations.

(c) Make a log-log plot of the production rate of CO_2 versus gas-phase CO concentration at constant gas-phase O_2 concentration. What are the slopes of the production rate at high and low CO concentrations?