Exam Advanced Chemical Reactor Engineering 6CPT30

April 3rd 2017

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Date: Monday, March 13th, 2017
Time: 9:00—12:00
Place: STC0.01

- There are two assignments of 5 points each. Points per subpart of the assignments are indicated.
- You are allowed to use a pen, pencil, rubber, ruler, and (graphic) calculator.
- Write your name and student ID on every paper you hand in.
- If you use more than one paper for an assignment, indicate the assignment number on the new paper and the subpart you are continuing, e.g. "2e) continued".
- No talking, for questions raise your hand.
- Switch off your mobile phone(s).

At 12:00 the exam ends. Hand in your papers and leave the room quietly. Some students are allowed to work longer. If you finish earlier, hand in your exam and leave the room discretely.

Success!
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Assignment 1: Reactor Selection (5 points)

General information

Consider the following reactors/catalyst combinations:

A. A trickle bed reactor with cylindrical particles of $d_p = 2$ mm, $h_p = 5$ mm, and eggshell distribution, $\delta_{eggshell} = 100$ μm. The catalyst loading is 1 wt% of Ru/C, the bed porosity is $\epsilon_b = 0.4$ $m^3_{void}/m^3_{reactor}$, and the mass transfer coefficients are: $k_{gl}a_{gl} = 0.1$ $m^3_L/m^3_{reactor}/s$, $k_{ls} = 5 \cdot 10^{-4}$ $m^3_L/m^2_i/s$. There is no direct gas-solid contact.

B. A 200 cpsi monolith with a catalyst layer of 10 μm, and a loading of 5 wt% Ru/C. The mass transfer coefficients are: $k_{gl}a_{gl} = 1$ $m^3_L/m^3_{reactor}/s$, $k_{ls}a_{ls} = 1$ $m^3_L/m^3_{reactor}/s$.

C. A slurry bubble column, with 10 % of the reactor volume occupied by 50 μm spherical particles of 5 wt% Ru/C. The gas holdup is 0.2, uniformly distributed in the reactor as small 6 mm diameter gas bubbles. The mass transfer coefficients are: $k_{gl} = 0.02$ $m^3_L/m^2_i/s$, $k_{ls} = 1.2$ $m^3_L/m^2_i/s$.

D. A mechanically stirred batch reactor with the same operating conditions of reactor C.

Motivate your answers as *quantitative*, as *complete*, and as *concise* as possible. Wrong comments/arguments will cost you points, even when the final answer is correct. Answers without motivation are not graded.

Questions:

a) Rank these combinations in terms of catalyst efficiency (1 point).

b) Rank the reactors by size for a mass transfer limited situation (1 point).

c) Rank the reactor by size for a kinetically limited situation (1 point).

d) Consider the pseudo-first order oxidation of liquid A using air as oxidant. For this reaction, $r_A = k_w \cdot C_{O_2}$ with $k_w = 100$ $m^3_L/s/kg_{Ru}$; catalyst density, $\rho_C = 2000$ $\text{kg}_{cat}/\text{m}^3_{cat}$. Rank the reactors for the highest conversion of A (1 point).

e) Rank the reactors for the highest possible selectivity for product B, given the reaction $A \rightarrow B$ with kinetics $r_B = k_r \cdot C_A$, and the undesired parallel reaction $A \rightarrow C$ with kinetics $r_C = k_r \cdot C_A$ (1 point).

Note: The Thiele Modulus for a first order reaction is given by: $\phi_{sphere} = R/3\sqrt{k_v/D_{eff}}$; $\phi_{cylinder} = R/2\sqrt{k_v/D_{eff}}$ (infinitely long cylinder) ; $\phi_{slab} = L\sqrt{k_v/D_{eff}}$; general $\phi = \frac{1}{a_{cat}}\sqrt{\frac{k_v}{D_{eff}}}$; $\eta = \tanh(\phi)/\phi$

Assignment 2: Transient behavior (5 points)

In this assignment you are asked to evaluate a number of transient situations. Carefully derive equations step-by-step.

Define each variable or parameter by name and specify the phase-specific units. So, if you need additional data/parameters, define these yourself, do not ask for these.

For each mole balance show that the units of the different terms match.

a) Consider a fluidized bed in which solid carbon particles react with CO_2: $C(s) + CO_2(g) \rightarrow 2CO(g)$. The reaction occurs at the gas-particle interface only and is first order in CO_2. The mass transfer coefficient is proportional to the square root of the particle radius.
Derive an equation that describes how the radius of a carbon particle changes in time as a function of the CO_2 concentration in the gas-particle emulsion phase.(2 points)

b) Consider a well stirred batch reactor in which liquid A is oxidized to liquid B with the help of a porous particle that supports a catalyst. The reaction is first order in A and in oxygen. The reactor is operated as follows:

1) The reactor is evacuated to complete vacuum.
2) Pure liquid A, concentration 12 mol/L is fed to the reactor until the reactor is filled for 50% of its total volume.
3) The catalyst is added to the system and the system is heated to the reaction temperature of 400 K.
4) The reactor is immediately pressurized with 21 vol% oxygen in nitrogen to a pressure that gives 0.95 times the stoichiometric amount of oxygen needed for completion of the reaction.
5) The stirrer is switched on. Assume that the gas-liquid mass transfer was negligible at zero stirring speed.

Derive an equation that gives the concentration of A as a function of time, starting from 5). Assume that gas-liquid mass transfer is the rate limiting step and that the gas behaves ideally. The vapour pressures of A and B are negligibly small. (3 points)

$A + O_2 \rightarrow C$

$A + 0{,}95\, O_2 \rightarrow C$

$\frac{d\, C_A \cdot V_R}{dt} = k \cdot C_{O_2} \cdot C_A \cdot V_R$

$\frac{m_l^3}{mol\, s}$ $\frac{mol}{m^3}$

$p \cdot V = n R T$

$k_{gl} \cdot a_{gl}$

$k_{gl} \cdot a_{gl} \cdot (P_{H_2} \cdot C_{O_2,sat} - C_{O_2,l}) \cdot V_R$

$\frac{m^3_l}{m^3_R\, s}$ $\frac{mol}{m^3_l}$

$P_{H_2} = \frac{nRT}{V}$ d