Exam Advanced Chemical Reactor Engineering 6CPT30

Date: Monday, March 7th, 2016
Time: 9:00 –12:00
Place: AUD14

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 quietly, leave the room quietly. No talking is allowed. If you finish earlier, hand in your exam and leave the room discretely.

Success!

1. Slurry bubble column (5 points in total)

We want to design a reactor for a hydrogenation rection: the heterogeneously catalyzed hydrogenation of dichloroacetic acid, an impurity in the desired product monochloroacetic acid: $H_2 + AcCl_2 \Longrightarrow AcCl + HCl$. The reaction rate in the porous catalyst particles is first order in hydrogen and in $AcCl_2$:

$$-r_{AcCl2} = k_r \cdot C_{H2} \cdot C_{AcCl2} \quad \text{in units } mol_{AcCl2} \cdot g_{Pt}^{-1} \cdot s^{-1}$$

The inlet flow of the process consists of 0.03 mole fraction of $AcCl_2$ in pure AcCl. The reaction product HCl diffuses back into the gas phase. Thus, although pure hydrogen is fed into the reactor, the gas phase is not pure hydrogen. The properties of the catalyst particles, gas, liquid, and the foreseen dimensions and operating conditions of the slurry bubble column process are listed below.

Assumptions:

1) The volumetric change in the gas phase by the reaction is negligible.
2) The ideal gas law applies.
3) A steady state condition is present in the slurry bubble column.
4) The gas bubble phase moves as a plug flow through the slurry bubble column.
5) The liquid phase with catalyst particles is ideally stirred.
6) No internal mass transfer limitation in the catalyst particle.
7) $AcCl_2$ and AcCl do not evaporate.
8) None of the components adsorb onto the particle.

The mass transfer to the catalyst particles in the liquid phase is given by (u_g is superficial gas velocity):

$$Sh_p = 2 + 0.47 \cdot Re_p^{0.66} \cdot Sc^{0.33} \quad \text{with} \quad Sh_p = \frac{k_{ls} \cdot d_p}{D_l} \quad Re_p = \frac{\rho_l \cdot E_d^{0.33} \cdot d_p^{1.33}}{\mu_l} \quad Sc = \frac{\mu_l}{\rho_l \cdot D_l} \quad E_d = g \cdot u_g$$

The overall mass transfer from gas to liquid phase is given by: $k_{gl} = 0.42 \cdot \left(\frac{g \cdot \mu_l}{\rho_l}\right)^{0.33} \cdot \left(\frac{D_l \cdot \rho_l}{\mu_l}\right)^{0.5}$ $\quad m_l^3 \cdot m_i^{-2} \cdot s^{-1}$

Questions:

a) What is the unit of k_r? What is the total gas-liquid interfacial area per volume in the reactor? (0.25 points)

b) Set up a mole balance for all relevant components in all relevant phases. (2 points)

c) How large should the hydrogen inlet flow be in mol/s to have a conversion of H_2 at the exit of 90% at steady state conditions, if the target concentration of $AcCl_2$ in the exit flow is 10 ppm (i.e., the mole fraction equals 10^{-5})? What is the corresponding volumetric flow rate of gas? (Assume $\phi_g = 1.5\ m_g^3 \cdot s^{-1}$ if you cannot calculate this value. This value is not necessarily the right answer!). (0.25 points)

d) Determine the rate limiting step. (0.75 points)

e) Use the rate limiting step result to derive an equation that gives the conversion of $AcCl_2$ as a function of slurry bubble column volume. (If you cannot find one rate limiting step, assume that gas to liquid mass transfer of H2 is limiting. Again: this is not necessarily the correct answer!) (0.75 points)

f) Calculate the needed slurry bubble column volume. (0.25 points)

g) How would you decrease the required volume of the slurry bubble column by a factor 100? Give quantitative arguments! What reactor would you choose if you could freely choose? (0.75 points)

Available data:

Diameter column	$D_R := 4.2$	m
Pressure	$p_R := 2.0$	bar
Temperature	$T_R := 400$	K
Catalyst particle diameter	$d_{cat} := 30 \cdot 10^{-6}$	m
Catalyst particle density	$\rho_{cat} := 1.5 \cdot 10^{3}$	$kg \cdot m^{-3}$
Catalyst particle loading with Pt	$L_{Pt} := 0.02$	$g_{Pt} \cdot g_{cat}^{-1}$
Catalyst particle concentration in liquid(!) (effect of catalyst on slurry density negligible)	$C_{cat} := 1$	$kg \cdot m_l^{-3}$
Liquid inlet flow	$\phi_l := 0.1$	$m_l^{3} \cdot s^{-1}$
Liquid viscosity	$\mu_l := 10^{-2}$	$Pa \cdot s$
Molecular weight AcCl	$M_{AcCl} := 0.095$	$kg \cdot mol^{-1}$
Molecular weight $AcCl_2$	$M_{AcCl2} := 0.129$	$kg \cdot mol^{-1}$
Density of AcCl and of $AcCl_2$	$\rho_{AcCl} := 1580$	$kg \cdot m_l^{-3}$
Diffusion coefficient of H_2 liquid phase	$D_{H2l} := 10^{-8}$	$m^2 s^{-1}$
Diffusion coefficient of $AcCl_2$ liquid phase	$D_{AcCl2} := 5 \cdot 10^{-10}$	$m^2 s^{-1}$
Gas fraction slurry bubble column	$\varepsilon_g := 0.15$	$m_g^{3} \cdot m_R^{-3}$
Gas bubble size	$d_b := 12 \cdot 10^{-3}$	m
Gas Viscosity	$\mu_g := 10^{-5}$	$Pa \cdot s$
Diffusion coefficient of H_2 gas phase	$D_{H2g} := 10^{-5}$	$m^2 s^{-1}$
Solubility H_2 in AcCl	$L_{H2} := 15$	$mol_{H2} \cdot m_l^{-3} \cdot bar_{H2}^{-1}$
Solubility HCl in AcCl	$L_{HCl} := 25$	$mol_{HCl} \cdot m_l^{-3} \cdot bar_{HCl}^{-1}$
Molecular weight of HCl	$M_{HCl} := 36 \cdot 10^{-3}$	$kg \cdot mol^{-1}$
Gas constant	$R := 8.314$	$J \cdot mol^{-1} \cdot K^{-1}$
Reaction rate constant	$k_r := 100$	?
Gravitational acceleration:	$g := 9.81$	$m \cdot s^{-2}$

2. Reactor Selection (5 points)

Consider the following reactors and catalysts:

A) 25 μm diameter spherical particle with uniform 4 wt% catalyst loading in a slurry bubble column (20 vol% solids in reactor), $k_l \cdot a_l = 0.25\ m_l^{3} \cdot m_R^{-3} \cdot s^{-1}$, $k_{ls} = 10^{-4}\ m_l^{3} \cdot m_{interface}^{-2} \cdot s^{-1}$.

B) 1 mm diameter spherical particle with 50 μm eggshell 1 wt% catalyst loading in a trickle bed, $k_{gl} \cdot a_{gl} = 1\ m_l^{3} \cdot m_R^{-3} \cdot s^{-1}$, $k_{ls} = 10^{-4}\ m_l^{3} \cdot m_{interface}^{-2} \cdot s^{-1}$. No direct gas to solid mass transfer.

C) 200 cpsi (1.5 mm channel width) monolith catalyst with 5 μm washcoat with 9 wt% uniform catalyst loading, $k_{gl} \cdot a_{gl} = 5\ m_l^{3} \cdot m_R^{-3} \cdot s^{-1}$, $k_{ls} = 10^{-4}\ m_l^{3} \cdot m_{interface}^{-2} \cdot s^{-1}$. No direct gas to solid mass transfer.

Motivate the answers as quantitative as possible to the questions. There is no word limit but be as concise as possible, wrong comments/arguments will cost you points, even if your final answer is correct. (1 point total for the correct ranking and motivation).

a. Rank the reactors / catalyst in order for the highest catalyst efficiency for a first order reaction which is effected by internal particle mass transfer limitation (do not take the reactor residence time distribution into account for this).

b. Rank the reactors for the highest possible selectivity for product (B) given the reaction A -> B with kinetics $r_B = k_r \cdot C_A^{-0.5}$ and the undesired parallel reaction A -> C with kinetics $r_C = k_r \cdot C_A$. The reaction is slow and external and internal mass transfer can be neglected.

c. Rank the reactors by size for a gas-liquid-solid mass transfer limited situation.

d. Rank the reactors by size for a kinetically limited case, first order reaction.

e. Give for all three reactors at least two ways (quantitative!) to increase the productivity by a factor 1.2, using all the data given in the description and with internal mass transfer limitations absent.

Note: The Thiele modulus for a first order reaction is given by:

$$\phi_{sphere} = \frac{R}{3} \cdot \sqrt{\frac{k_r}{D}} \qquad \phi_{cylinder} = \frac{R}{2} \cdot \sqrt{\frac{k_r}{D}} \qquad \phi_{slab} = L \cdot \sqrt{\frac{k_r}{D}}$$