

# **Exam Advanced Chemical Reactor Engineering 6CPT30**

Date: Monday, March 7<sup>th</sup>, 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 reaction: the heterogeneously catalyzed hydrogenation of dichloroacetic acid, an impurity in the desired product monochloroacetic acid:  $\text{H}_2 + \text{AcCl}_2 \rightleftharpoons \text{AcCl} + \text{HCl}$ . The reaction rate in the porous catalyst particles is first order in hydrogen and in  $\text{AcCl}_2$ :

$$-r_{\text{AcCl}_2} = k_f \cdot C_{\text{H}_2} \cdot C_{\text{AcCl}_2} \quad \text{in units } \text{mol}_{\text{AcCl}_2} \cdot \text{g}_{\text{Pt}}^{-1} \cdot \text{s}^{-1}$$

The inlet flow of the process consists of 0.03 mole fraction of  $\text{AcCl}_2$  in pure  $\text{AcCl}$ . The reaction product  $\text{HCl}$  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)  $\text{AcCl}_2$  and  $\text{AcCl}$  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):

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

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

### Questions:

- a) What is the unit of  $k_f$ ? 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  $\text{H}_2$  at the exit of 90% at steady state conditions, if the target concentration of  $\text{AcCl}_2$  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  $\phi_g = 1.5 \text{ m}_g^3 \cdot \text{s}^{-1}$  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  $\text{AcCl}_2$  as a function of slurry bubble column volume. (If you cannot find one rate limiting step, assume that gas to liquid mass transfer of  $\text{H}_2$  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	$\rho_{cat} := 1.5 \cdot 10^3$	$\text{kg} \cdot \text{m}^{-3}$
Catalyst particle loading with Pt	$L_{Pt} := 0.02$	$\text{g}_{Pt} \cdot \text{g}_{cat}^{-1}$
Catalyst particle concentration in liquid(!) (effect of catalyst on slurry density negligible)	$C_{cat} := 1$	$\text{kg} \cdot \text{m}_l^{-3}$
Liquid inlet flow	$\phi_l := 0.1$	$\text{m}_l^3 \cdot \text{s}^{-1}$
Liquid viscosity	$\mu_l := 10^{-2}$	Pa·s
Molecular weight AcCl	$M_{AcCl} := 0.095$	$\text{kg} \cdot \text{mol}^{-1}$
Molecular weight AcCl <sub>2</sub>	$M_{AcCl_2} := 0.129$	$\text{kg} \cdot \text{mol}^{-1}$
Density of AcCl and of AcCl <sub>2</sub>	$\rho_{AcCl} := 1580$	$\text{kg} \cdot \text{m}_l^{-3}$
Diffusion coefficient of H <sub>2</sub> liquid phase	$D_{H_2l} := 10^{-8}$	$\text{m}^2 \cdot \text{s}^{-1}$
Diffusion coefficient of AcCl <sub>2</sub> liquid phase	$D_{AcCl_2} := 5 \cdot 10^{-10}$	$\text{m}^2 \cdot \text{s}^{-1}$
Gas fraction slurry bubble column	$\epsilon_g := 0.15$	$\text{m}_g^3 \cdot \text{m}_R^{-3}$
Gas bubble size	$d_b := 12 \cdot 10^{-3}$	m
Gas Viscosity	$\mu_g := 10^{-5}$	Pa·s
Diffusion coefficient of H <sub>2</sub> gas phase	$D_{H_2g} := 10^{-5}$	$\text{m}^2 \cdot \text{s}^{-1}$
Solubility H <sub>2</sub> in AcCl	$L_{H_2} := 15$	$\text{mol}_{H_2} \cdot \text{m}_l^{-3} \cdot \text{bar}_{H_2}^{-1}$
Solubility HCl in AcCl	$L_{HCl} := 25$	$\text{mol}_{HCl} \cdot \text{m}_l^{-3} \cdot \text{bar}_{HCl}^{-1}$
Molecular weight of HCl	$M_{HCl} := 36 \cdot 10^{-3}$	$\text{kg} \cdot \text{mol}^{-1}$
Gas constant	$R := 8.314$	$\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$
Reaction rate constant	$k_r := 100$	?
Gravitational acceleration:	$g := 9.81$	$\text{m} \cdot \text{s}^{-2}$

## 2. Reactor Selection (5 points)

Consider the following reactors and catalysts:

A) 25  $\mu\text{m}$  diameter spherical particle with uniform 4 wt% catalyst loading in a slurry bubble column (20 vol% solids in reactor),  $k_{gl} \cdot a_{gl} = 0.25 \text{ m}_l^3 \cdot \text{m}_R^{-3} \cdot \text{s}^{-1}$ ,  $k_{ls} = 10^{-4} \text{ m}_l^3 \cdot \text{m}_{\text{interface}}^{-2} \cdot \text{s}^{-1}$ .

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

C) 200 cpsi (1.5 mm channel width) monolith catalyst with 5  $\mu\text{m}$  washcoat with 9 wt% uniform catalyst loading,  $k_{gl} \cdot a_{gl} = 5 \text{ m}_l^3 \cdot \text{m}_R^{-3} \cdot \text{s}^{-1}$ ,  $k_{ls} = 10^{-4} \text{ m}_l^3 \cdot \text{m}_{\text{interface}}^{-2} \cdot \text{s}^{-1}$ . 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).

- 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).
- Rank the reactors for the highest possible selectivity for product (B) given the reaction  $A \rightarrow B$  with kinetics  $r_B = k_f \cdot C_A^{-0.5}$  and the undesired parallel reaction  $A \rightarrow C$  with kinetics  $r_C = k_f \cdot C_A$ . The reaction is slow and external and internal mass transfer can be neglected.
- Rank the reactors by size for a gas-liquid-solid mass transfer limited situation.
- Rank the reactors by size for a kinetically limited case, first order reaction.
- 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:

$$\phi_{\text{sphere}} = \frac{R}{3} \cdot \sqrt{\frac{k_f}{D}} \quad \phi_{\text{cylinder}} = \frac{R}{2} \cdot \sqrt{\frac{k_f}{D}} \quad \phi_{\text{slab}} = L \cdot \sqrt{\frac{k_f}{D}}$$

Answer 2. Reactor selection

Overview of data:

	A. SBC	B. TBR	C. Monolith
Thiele modulus	$\frac{25}{6} \cdot \sqrt{4} = 8.333$	$50 \cdot \sqrt{1} = 50$	$5 \cdot \sqrt{9} = 15$
$k_{gl} \cdot a_{gl}$	0.25	1	5
$\epsilon_{cat}$	0.2	$0.6 \cdot 50 \cdot 10^{-6} \cdot \frac{6}{10^{-3}} = 0.18$	$\frac{5 \cdot 10^{-6} \cdot 4 \cdot 1.5 \cdot 10^{-3}}{(1.8 \cdot 10^{-3})^2} = 9.259 \times 10^{-3}$
$a_s$	$\frac{6 \cdot 0.2}{25 \cdot 10^{-6}} = 4.8 \times 10^4$	$\frac{6 \cdot 0.6}{10^{-3}} = 3.6 \times 10^3$	$\frac{4 \cdot 1.5 \cdot 10^{-3}}{(1.8 \cdot 10^{-3})^2} = 1.852 \times 10^3$
$k_{ls} \cdot a_{ls}$	$10^{-4} \cdot \frac{6 \cdot 0.2}{25 \cdot 10^{-6}} = 4.8$	$10^{-4} \cdot \frac{6 \cdot 0.6}{10^{-3}} = 0.36$	$10^{-4} \cdot \frac{4 \cdot 1.5 \cdot 10^{-3}}{(1.8 \cdot 10^{-3})^2} = 0.185$
$L_{cat} \cdot \epsilon_{cat}$	$0.2 \cdot 4 = 0.8$	$0.18 \cdot 1 = 0.18$	$9.259 \cdot 10^{-3} \cdot 9 = 0.083$
$k_{ovl}$	$\left(\frac{1}{0.25} + \frac{1}{4.8}\right)^{-1} = 0.238$	$\left(\frac{1}{1} + \frac{1}{0.36}\right)^{-1} = 0.265$	$\left(\frac{1}{5} + \frac{1}{0.185}\right)^{-1} = 0.178$
RTD	Well mixed, no dead volume in particles (small)	~ideal PFR, dead volume in particles	ideal PFR, no dead volume (thin washcoat)

a) We are looking for the lowest Thiele modulus, this gives the highest efficiency, see Scott Fogler. The  $k_r$  in the

Thiele modulus is the volumetric reaction rate constant in units  $s^{-1}$ . The reaction rate for the pseudo first order reaction depends on the catalyst concentration, and is given by:

$$-r_A = k_{cat} \cdot L_{cat} \cdot \rho_p \cdot c_A = k_r \cdot c_A \text{ with } (L_{cat} \cdot \rho_p) \text{ in units } g_{cat} \cdot m_p^{-3} \text{ and } k_{cat} \text{ in } m_p^3 \cdot g_{cat}^{-1} \cdot s^{-1}$$

Then we get for the three options, taking only the varying parameters (size, shape, and loading) into account:

A: spherical so:  $\frac{25}{6} \cdot \sqrt{4} = 8.333$

B: eggshell is approximately flat plate geometry:  $50 \cdot \sqrt{1} = 50$

C: flat plate geometry  $5 \cdot \sqrt{9} = 15$

Thus  $A > C > B$

b) The selectivity is determined by the rate of the desired reaction over the rate of the undesired reaction, i.e.

$$S = \frac{k_r \cdot C_A^{-0.5}}{k_r \cdot C_A} = \frac{1}{C_A^{1.5}}$$

Thus, for the highest selectivity we want the lowest concentration of A. Therefore we want

ideally mixed behavior. The SBC will perform best, then the TBR (non-ideal PFR), and then the MR.

c) For this case, we need to look at  $k_{ovl}$  and flow behavior. The TBR has the highest value combined with plug flow behavior, the conversion of gas is  $X_{TBR} = 1 - \exp(-k_{ovl} \cdot \tau)$ .  $k_{ovl}$  is per volume of reactor, so  $\tau$  is based on reactor volume. Because the mass transfer of the TBR is higher than the SBC, the TBR is always better. For the monolith it is not that simple. The selection depends on the desired conversion. We can see that in the graph below in which the conversion for the different reactors is plotted.

$kt := 0.01, 0.02 \dots 40$

The conversion for the SBC is:

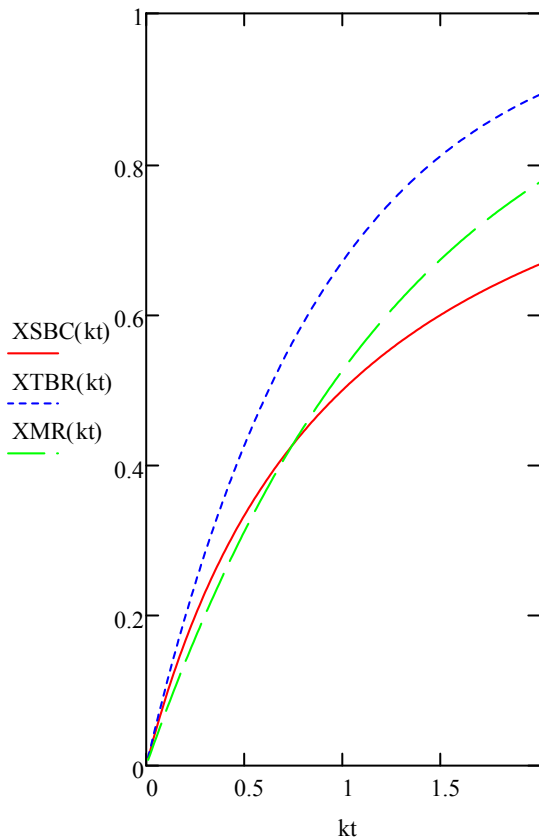
$$XSBC(k\tau) := \frac{k\tau}{1 + k\tau}$$

The corresponding conversion for an ideal PFR TBR is (corrected for different  $k_{ovl}$ ):

$$XTBR(k\tau) := 1 - \exp\left(\frac{-0.265}{0.238} \cdot k\tau\right)$$

The corresponding conversion for an ideal PFR MR is (corrected for different  $k_{ovl}$ ):

$$XMR(k\tau) := 1 - \exp\left(\frac{-0.178}{0.238} \cdot k\tau\right)$$



We see that for  $kt$  below  $\sim 0.75$ , ( $X \sim 0.4$ ), the conversion of the SBC is higher than for the monolith. So, if the desired conversion is above 0.4, a MR gives a lower volume than a SBC!

$X > 0.4$ : volume of TBR < MR < SBC  
 $X \leq 0.4$ : volume of TBR < SBC < MR

c) For a kinetically limited case we need to look at  $\epsilon_{\text{cat}} \cdot L_{\text{cat}}$  in a similar way as above:

The conversion for the SBC is:

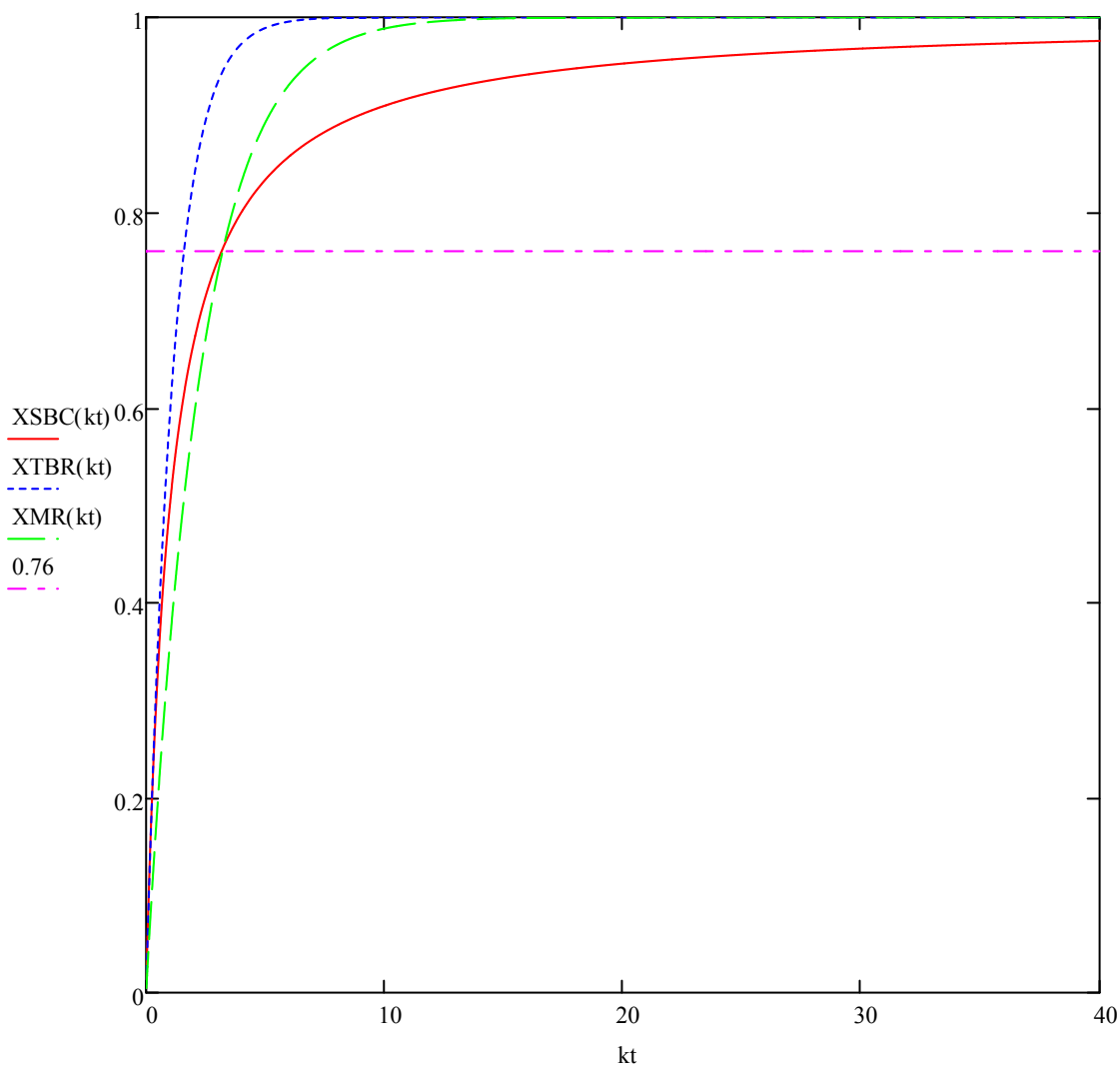
$$X_{\text{SBC}}(k\tau) := \frac{k\tau}{1 + k\tau}$$

The corresponding conversion for an ideal PFR TBR  
is (corrected for different solids holdup and catalyst loading):

$$X_{\text{TBR}}(k\tau) := 1 - \exp\left(\frac{-0.18}{0.2} \cdot k\tau\right)$$

The corresponding conversion for an ideal PFR MR  
is (corrected for different solids holdup and catalyst loading):

$$X_{\text{MR}}(k\tau) := 1 - \exp\left(\frac{-0.089}{0.2} \cdot k\tau\right)$$



Again we find that the TBR performs best and the choice between MR and SBC depends on conversion, for conversions above  $\sim 0.76$  (see graph), the MR volume is less than the SBC volume.

Answers 1. SBC (5 pts)

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

$$m_{l\_cat} \cdot 6 \cdot \text{mol}_{H_2}^{-1} \cdot \text{g}_{Pt}^{-1} \quad \text{where } m_{l\_cat} \text{ is the liquid inside the porous catalyst particle}$$

$$a_{gl} := \frac{6 \cdot \epsilon_g}{d_b} = 75 \quad m_i^2 \cdot m_R^{-3}$$

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

$$A_R := \frac{\pi}{4} \cdot D_R^2 = 13.854 \quad m_R^2$$

H2 balance gas phase:

$$0 = \left( y_{H_2} \cdot \frac{\phi_g \cdot P_R \cdot 10^5}{R \cdot T_R} \right)^z - \left( y_{H_2} \cdot \frac{\phi_g \cdot P_R \cdot 10^5}{R \cdot T_R} \right)^{z+\Delta z} - k_{gl} \cdot a_{gl} \cdot A_R \cdot \Delta z \cdot (y_{H_2} \cdot P_R \cdot L_{H_2} - C_{H_2l}) \quad P_R \text{ in bar!}$$

H2 balance liquid phase:

$$0 = \phi_l \cdot C_{H_2l\_in} - \phi_l \cdot C_{H_2l} + \int_0^{H_R} k_{gl} \cdot a_{gl} \cdot A_R \cdot (y_{H_2}(z) \cdot P_R \cdot L_{H_2} - C_{H_2l}) dz - k_{ls} \cdot a_{ls} \cdot (C_{H_2l} - C_{H_2p}) \cdot A_R \cdot H_R$$

H2 balance catalyst particle:

$$0 = 0 - 0 + k_{ls} \cdot a_{ls} \cdot (C_{H_2l} - C_{H_2p}) \cdot A_R \cdot H_R - k_r \cdot \eta \cdot L_{Pt} \cdot C_{cat} \cdot (1 - \epsilon_g) \cdot A_R \cdot H_R \cdot C_{H_2p} \cdot C_{AcCl_2p}$$

HCl balances:

$$0 = \left( y_{HCl} \cdot \frac{\phi_g \cdot P_R \cdot 10^5}{R \cdot T_R} \right)^z - \left( y_{HCl} \cdot \frac{\phi_g \cdot P_R \cdot 10^5}{R \cdot T_R} \right)^{z+\Delta z} - k_{gl} \cdot a_{gl} \cdot A_R \cdot \Delta z \cdot (y_{HCl} \cdot P_R \cdot L_{HCl} - C_{HCl l})$$

$$0 = \phi_l \cdot C_{HCl l\_in} - \phi_l \cdot C_{HCl l} + \int_0^{H_R} k_{gl} \cdot a_{gl} \cdot A_R \cdot (y_{HCl}(z) \cdot P_R \cdot L_{HCl} - C_{HCl l}) dz - k_{ls} \cdot a_{ls} \cdot (C_{HCl l} - C_{HCl p}) \cdot A_R \cdot H_R$$

$$0 = 0 - 0 + k_{ls} \cdot a_{ls} \cdot (C_{HCl l} - C_{HCl p}) \cdot A_R \cdot H_R + k_r \cdot \eta \cdot L_{Pt} \cdot C_{cat} \cdot (1 - \epsilon_g) \cdot A_R \cdot H_R \cdot C_{H_2p} \cdot C_{AcCl_2p}$$

Dichloroacetic acid balances:

$$0 = \phi_l \cdot C_{AcCl_2\_in} - \phi_l \cdot C_{AcCl_2} - k_{ls} \cdot a_{ls} \cdot (C_{AcCl_2l} - C_{AcCl_2p}) \cdot A_R \cdot H_R$$

$$0 = 0 - 0 + k_{ls} \cdot a_{ls} \cdot (C_{AcCl_2l} - C_{AcCl_2p}) \cdot A_R \cdot H_R - k_r \cdot \eta \cdot L_{Pt} \cdot C_{cat} \cdot (1 - \epsilon_g) \cdot A_R \cdot H_R \cdot C_{H_2p} \cdot C_{AcCl_2p}$$



c) How large should the hydrogen inlet flow be in mol/s to have a conversion of H<sub>2</sub> at the exit of 90%? What is the corresponding volumetric flow rate of gas? (Assume  $\phi_g = 1.5 \text{ m}_g^3 \cdot \text{s}^{-1}$  if you cannot calculate this value. This value is not necessarily the right answer). (0.25 points)

The consumption of H<sub>2</sub> is given by the target conversion:

$$x_{\text{AcCl}} := 1 - 10^{-5} \quad C_{\text{tot}} := \left[ x_{\text{AcCl}} \cdot \frac{M_{\text{AcCl}}}{\rho_{\text{AcCl}}} + (1 - x_{\text{AcCl}}) \cdot \frac{M_{\text{AcCl}_2}}{\rho_{\text{AcCl}}} \right]^{-1} = 1.663 \times 10^4 \text{ mol}_{\text{tot}} \cdot \text{m}_L^{-3}$$

$$\phi_{\text{molAcCl}_2} := \phi_1 \cdot C_{\text{tot}} \cdot (0.03 - 10^{-5}) = 49.878 \text{ mol}_{\text{AcCl}_2} \cdot \text{s}^{-1}$$

At the given conditions the volumetric gas flow rate is:

$$\phi_g := \frac{1}{0.9} \cdot \phi_{\text{molAcCl}_2} \cdot \frac{R \cdot T_R}{p_R \cdot 10^5} = 0.922 \text{ m}^3 \cdot \text{s}^{-1} \quad u_g := \frac{\phi_g}{A_R} = 0.067 \text{ m}_g^3 \cdot \text{m}_R^{-2} \cdot \text{s}^{-1}$$

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

Compare different terms at maximum driving forces (only reactants H<sub>2</sub> and AcCl<sub>2</sub> important):

H<sub>2</sub> gas liquid:

$$C_{\text{H}_2\text{lmax}} := 1 \cdot p_R \cdot L_{\text{H}_2} = 30 \text{ mol} \cdot \text{m}_l^{-3}$$

$$k_{\text{gl}} := 0.42 \cdot \left( \frac{\text{g} \cdot \mu_l}{\rho_{\text{AcCl}}} \right)^{0.33} \cdot \left( \frac{D_{\text{H}_2\text{l}} \cdot \rho_{\text{AcCl}}}{\mu_l} \right)^{0.5} = 6.828 \times 10^{-4} \text{ m}_l^3 \cdot \text{m}_i^{-2} \cdot \text{s}^{-1}$$

$$k_{\text{gl}} \cdot a_{\text{gl}} \cdot C_{\text{H}_2\text{lmax}} = 1.536 \text{ mol} \cdot \text{m}_R^{-3} \cdot \text{s}^{-1} \quad k_{\text{gl}} \cdot a_{\text{gl}} = 0.051$$

H<sub>2</sub> liquid-solid:

$$E_d := \frac{\text{g} \cdot \phi_g}{A_R} = 0.653 \text{ W} \cdot \text{m}_l^{-3} \quad Sc := \frac{\mu_l}{\rho_{\text{AcCl}} \cdot D_{\text{H}_2\text{l}}} = 632.911 \quad Re_p := \frac{\rho_{\text{AcCl}} \cdot E_d^{0.33} \cdot d_{\text{cat}}^{1.33}}{\mu_l} = 0.132$$

$$Sh_p := 2 + 0.47 \cdot Re_p^{0.66} \cdot Sc^{0.33} = 3.04 \quad k_{\text{ls}} := Sh_p \cdot \frac{D_{\text{H}_2\text{l}}}{d_{\text{cat}}} = 1.013 \times 10^{-3}$$

$$\text{total catalyst surface area in liquid:} \quad \epsilon_{\text{cat}} := \frac{C_{\text{cat}}}{\rho_{\text{cat}}} \cdot (1 - \epsilon_g) = 5.667 \times 10^{-4} \quad a_{\text{ls}} := \frac{6 \cdot \epsilon_{\text{cat}}}{d_{\text{cat}}} = 113.333 \quad k_{\text{ls}} \cdot a_{\text{ls}} = 0.115$$

$$k_{\text{ls}} \cdot a_{\text{ls}} \cdot C_{\text{H}_2\text{lmax}} = 3.445 \text{ mol} \cdot \text{m}_R^{-3} \cdot \text{s}^{-1}$$

H<sub>2</sub>/AcCl<sub>2</sub> reaction (note that the entire reactor operates on the exit concentration, not the inlet concentration!!!). The reactor concentration is:

$$C_{\text{AcCl}_2} := 10^{-5} \cdot \frac{\rho_{\text{AcCl}}}{M_{\text{AcCl}}} = 0.166 \quad \text{mol}_{\text{AcCl}_2} \cdot \text{m}_l^{-3} \quad \eta := 1$$

$$k_r \cdot \eta \cdot L_{\text{Pt}} \cdot C_{\text{cat}} \cdot (1 - \epsilon_g) \cdot C_{\text{H}_2 \text{max}} \cdot C_{\text{AcCl}_2} = 8.482 \quad \text{mol}_{\text{AcCl}_2} \cdot \text{m}_l^{-3}$$

All H<sub>2</sub> contributions are of the same order of magnitude and cannot be neglected. Now let's investigate AcCl<sub>2</sub> mass transfer (reaction is the same):

$$Sc := \frac{\mu_l}{\rho_{\text{AcCl}} \cdot D_{\text{AcCl}_2}} = 1.266 \times 10^4 \quad Sh_p := 2 + 0.47 \cdot Re_p^{0.66} \cdot Sc^{0.33} = 4.795 \quad k_{ls} := Sh_p \cdot \frac{D_{\text{AcCl}_2}}{d_{\text{cat}}} = 7.992 \times 10^{-5}$$

$$k_{ls} \cdot a_{ls} \cdot C_{\text{AcCl}_2} = 1.506 \times 10^{-3} \quad \text{mol} \cdot \text{m}_R^{-3} \cdot \text{s}^{-1}$$

This is more than 10x less than the smallest H<sub>2</sub>-mole flow (even if y<sub>H2</sub>=0.9 is assumed) and therefore the rate limiting step! The concentration in the particle is therefore approximately zero.

e) The balance is now simple: (0.75 pts)

$$0 = \phi_l \cdot C_{\text{AcCl}_2 \text{in}} - \phi_l \cdot C_{\text{AcCl}_2} - k_{ls} \cdot a_{ls} \cdot (C_{\text{AcCl}_2} - C_{\text{AcCl}_2p}) \cdot V_R$$

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

$$V_R := \frac{\phi_{\text{molAcCl}_2}}{k_{ls} \cdot a_{ls} \cdot C_{\text{AcCl}_2}} = 3.311 \times 10^4 \quad \text{m}_R^3 \quad H_R := \frac{V_R}{A_R} = 2.39 \times 10^3 \quad \text{m}_R$$

Clearly this is an enormous reactor which would never be built. The 'intensification' with a factor 100 is a must!

g) How would you improve the productivity while still using the slurry bubble column?

What reactor would you choose if you could change? (0.5 points)

We need to increase the catalyst concentration by at least a factor 100, the rate limiting step then increases with the same factor and becomes 0.15, still a factor 10 smaller than the hydrogen gas-liquid RLS. This GL mass transfer could be augmented by increasing gas velocity or the pressure of the reactor.

Much lesser volume of the reactor could be obtained with a plug flow reactor with a lot of catalyst: a trickle bed reactor. The difference in volume between a PFR(TBR) and a CSTR(SBC) becomes huge at high conversions. The higher catalyst loading adds to this.



