# Exam Advanced Chemical Reactor Engineering 6CPT30

Date: Friday, April 15th, 2016
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 quietly, leave the room quietly. No talking is allowed. If you finish earlier, hand in your exam and leave the room discretely.

Success!

Assignment 1: Trickle-Bed Reactor

In a pilot plant, a trickle-bed reactor (TBR) is used to conduct the hydrogenation of a hydrocarbon (A) over a palladium on alumina catalyst. Because typically the mass transfer of hydrogen from the gas phase to the catalyst surface is very slow, the engineer in charge decided to operate the reactor with a high hydrogen pressure, and large catalyst particles to reduce pressure drop. Although TBR usually suffer from important pressure drops, in this case it can be assumed that the pressure drop does not have any significant effect on the reactor performance. The catalyst particles are cylindrical with an eggshell layer to reduce the intra-particle diffusion limitations. Pure hydrogen gas is fed co-currently with the liquid phase. It is assumed that both gas and liquid present ideal plug flow behavior, and that there is no film of static liquid around the catalyst particles. A fraction of the catalyst surface, $f_g$, is in contact with the gas, and the rest, $f_l$, is in contact with the liquid ($f_g + f_l = 1$).

The reaction rate is:

$$r = \eta k C_{H_2} \frac{K_A C_A}{1 + K_A C_A}$$

with:

$$\eta = \frac{tanh\phi}{\phi}$$

$$\phi = d_{egg-shell}\sqrt{k/D_{eff}}$$

**Data:**

$k$=2000 $s^{-1}$ (in the Pd on alumina egg-shell)
$K_A$=13.3 $m^3 mol^{-1}$
Effective diffusion coefficient, $D_{eff}$: $5 \cdot 10^{-9}$ $m^2/s$

Diameter of catalyst particle, $d_p$: 5 mm
Length of catalyst particle, $L$: 10 mm
Eggshell thickness, $d_{egg-shell}$: 100 $\mu$m
Bed porosity, $\epsilon_b$: 0.4 $m^3_{void}/m^3_{reactor}$

Superficial liquid velocity, $v_l$: 0.02 m/s
Superficial gas velocity, $v_g$: 0.20 m/s

Hydrogen pressure, P: 30 bar
Liquid inlet temperature, T: 323 K
Inlet concentration of A, $C_A$: 120 $mol/m^3_{liq}$
Saturation concentration of hydrogen, $C_{sat}$= 4 $mol/m^3_{liq}/bar$

# Assignment 2 Fluidized Beds (5 points in total)

Consider a fluidized bed combustor operated in the bubbling fluidization regime. In a fluidized bed of sand particles pure carbon particles are burnt with oxygen from air according to the following reaction:

$O_{2(g)} + C_{(s)} ==> CO_{2(g)}$

The volumetric change in the gas phase by the reaction is negligible. The sand particles are inert and are only present to buffer the heat and to efficiently transport the heat to the heat exchange tubes in the bed. The properties of the particles and the dimensions and operating conditions of the combustor are given below. Assume that the ideal gas law applies. The carbon particles are added to the fluidized bed of sand at start-up after the sand has been preheated to the operating temperature by the combustion of natural gas.

The reaction rate at the surface of a solid carbon particle is given by:

$$-r_C = k_r \cdot C_{O2g} \quad mol_C \cdot m_{surface}^{-2} \cdot s^{-1}$$

a) Explain in less than 100 words (>100 words=no points!) the physical background of fluidization. (If you are not proficient enough in English you may explain in Dutch). (0.25 points)

b) The fluidization behavior is determined by the sand particles. Determine the Geldart classification of the sand particles. (0.25 points)

c) Calculate the gas bubble fraction. Assume that the bed expands with a factor 1.33 and validate this assumption. Assume that the added carbon particles are well mixed in the bed and behave as though they were sand particles. (0.5 points)

Assume that the gas bubble phase is ideally stirred and that the particle emulsion phase is ideally stirred.

d) Set up a mole balance for oxygen in the gas bubble phase, the emulsion phase and the particle interface for a steady state. (1.0 points)

e) Show by dimension analysis that your mole balance is correct. Use phase specific units! (0.25 points).

f) Determine the rate limiting step(s) (0.5 points).

g) Calculate the conversion of oxygen if the carbon particles do not shrink due to reaction. What are the concentrations of oxygen in the bubble phase, the emulsion phase and the solid surface? (1.0 points)

h) How does the shrinking of the carbon particles influence your result? Explain! (0.25 points)

i) The gas phase flow is more correctly described as a plug flow. How are your results influenced by the assumption of ideally stirred gas bubble phase? (0.5 points)

Fraction of catalyst surface in contact with liquid, $f_l$= 0.11
Specific surface area, $a_{ls} = 4/d_p \cdot (1 - \epsilon_b) \cdot f_l$
Specific surface area, $a_{gs} = 4/d_p \cdot (1 - \epsilon_b) \cdot f_g$

Gas-liquid mass transfer coefficient, $k_{gl}a_{gl}$: $5{\cdot}10^{-2} \mathrm{m}^3_{liq}/\ \mathrm{m}^3_{reactor}\mathrm{s}$
Liquid-solid mass transfer coefficient, $k_{ls}$: $7{\cdot}10^{-4} \mathrm{m}^3_{liq}/\ \mathrm{m}^2_i\mathrm{s}$
Gas-solid mass transfer coefficient, $k_{gs}$: $8{\cdot}10^{-5} \mathrm{m}^3_{liq}/\ \mathrm{m}^2_i\mathrm{s}$

a) What is the length of the reactor needed to achieve 99% conversion of A? (3 points)

b) After a period of time, the activity of the catalyst has dropped due to the formation of gum on the surface of the catalyst. Effectively, this reduces the catalyst activity to 10% of its original activity. What is the length of the reactor needed to achieve 99% conversion of A in this case? (1 point)

c) We have assumed that the pressure drop along the reactor is negligible, but in fact, in a typical TBR the pressure drop is relatively high and cannot be neglected. What would be the effect of the pressure drop on the reactor performance? (1 point)

Combustor dimensions and operating conditions:

| | | |
|---|---|---|
| Diameter | $D_R := 0.8$ | m |
| Sand inventory | $m_{sand} := 1200$ | $kg_{sand}$ |
| Pressure | $p_R := 1.5 \cdot 10^5$ | Pa |
| Temperature | $T_R := 1000$ | K |
| Volumetric flow at T=273 K and p=1 bar | $\phi_v := 0.1$ | $m^3 s^{-1}$ |
| Mass of carbon added at start-up | $m_{carbon} := 50$ | $kg_{carbon}$ |

Particle properties:

| | | |
|---|---|---|
| Sand particle diameter | $d_{sand} := 0.1 \cdot 10^{-3}$ | m |
| Sand particle density | $\rho_{sand} := 2300$ | $kg \cdot m^{-3}$ |
| Carbon particle diameter | $d_{carbon} := 0.5 \cdot 10^{-3}$ | m |
| Carbon particle density | $\rho_{carbon} := 900$ | $kg \cdot m^{-3}$ |
| Gas fraction at minimum fluidization | $\varepsilon_{mf} := 0.42$ | $m_g{}^3 \cdot m_R{}^{-3}$ |

Gas phase properties:

| | | |
|---|---|---|
| Viscosity | $\mu_g := 10^{-5}$ | $Pa \cdot s$ |
| Diffusion coefficient of $O_2$ | $D_g := 10^{-6}$ | $m^2 s^{-1}$ |
| Average molecular weight of gas | $M_g := 30 \cdot 10^{-3}$ | $kg \cdot mol^{-1}$ |
| Gas constant | $R := 8.314$ | $J \cdot mol^{-1} \cdot K^{-1}$ |

Miscellaneous:

| | | |
|---|---|---|
| Reaction rate constant | $k_r := 100$ | $mol_C \cdot m_g{}^3 \cdot mol_{O2}{}^{-1} \cdot m_{surface}{}^{-2} \cdot s^{-1}$ |
| Gravitational acceleration: | $g := 9.81$ | $m \cdot s^{-2}$ |

Further data and formulae to be used:
Archimedes number:

$$Ar = \frac{d_p^3 \cdot \rho_g \cdot (\rho_p - \rho_g) \cdot g}{\mu_g^2}$$

The dimensionless particle diameter is: $d_{po} = Ar^{\frac{1}{3}}$

Geldart A particles have a gas bubble diameter of 2 cm. For Geldart B particles the bubble diameter is given by (h=0.4*$H_R$!):

$$d_b = (u_0 - u_{mf})^{0.5} \cdot h^{0.75} \cdot g^{-0.25}$$

The rise velocity of a gas bubble is: $u_b = u_0 - u_{mf} + u_{binf}$ with $u_{binf} = 0.71 \cdot \sqrt{g \cdot d_b}$

The volume fraction of bubbles is: $\varepsilon_b = \frac{u_0 - u_{mf}}{u_b}$

The mass transfer coefficent from the gas bubbles tot the emulsion phase is:

$$k_q = \frac{u_{mf}}{3} + \sqrt{\frac{4 \cdot D_g \cdot u_b}{\pi \cdot d_b}} \quad m_{gas}^3 \cdot m_{bubble}^{-2} \cdot s^{-1}$$

The mass transfer to the carbon particles in the emulsion phase is

$$Sh_p = 1.8 \cdot Re_{mf}^{\frac{1}{2}} \cdot Sc^{\frac{1}{3}} \quad \text{with} \quad Sh_p = \frac{k_E \cdot d_p}{D_g} \quad Re_{mf} = \frac{\rho_g \cdot u_{mf} \cdot d_p}{\mu_g} \quad Sc = \frac{\mu_g}{\rho_g \cdot D_g}$$

Note: the Sherwood and Reynolds number are based on the carbon particle diameter but the Reynolds number is calculated wit the $u_{mf}$ of the sand particles!

The boundaries for the Geldart particle classification (C-A-B-D) are:

$$Ar_{CA} := 1.2 \qquad Ar_{AB} := 1.03 \cdot 10^6 \cdot \left(\frac{\rho_g}{\rho_p - \rho_g}\right)^{1.275} \qquad Ar_{BD} := 1.25 \cdot 10^5$$

The minimum fluidization velocity is given by: $Re_{mf} := \sqrt{33.7^2 + 0.0408 \cdot Ar} - 33.7$

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