Exam Advanced Chemical Reactor Engineering 6CPT30

2 July 2018, 18:00h - 21:00h
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Instructions:

This exam contains two assignments of 5 points each. Points per subpart of the assignments are indicated after each question.

You are allowed to use a pen, pencil, rubber, ruler and a (non programmable) calculator.

Write your name and student number 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. For example, "2e) continued".

It is not allowed to talk during the exam. For questions, please raise your hand.

Switch off your mobile phone(s).

At 21:00 h the exam ends. Hand in your papers quietly and leave the room. If you finish your exam earlier, hand in your exam and leave the room discretely.

Success!

Assignment 1: Structured Reactor (5 points)

The conversion of biomass to useful chemicals is receiving increasing attention. One example is the conversion of X, a bio-based carbohydrate into F, a valuable chemical that is used in the production of pharmaceuticals, coatings, and many other industrial products. The conversion of X to F takes place via acid catalyzed dehydration in an aqueous solution at elevated temperature and pressure (note: the pressure is sufficiently high to maintain all the components in the liquid phase):

$$X(aq) \xrightarrow[k_{v1}]{\text{Acid catalyst}} F(aq) + 3\text{H}_2\text{O}$$

Unfortunately, under the same reaction conditions, F degrades to D, a waste product:

$$F(aq) \xrightarrow[k_{v2}]{\text{Acid catalyst}} D(aq)$$

With reaction rates equal to:

$$r_1 = \eta_1 k_{v1} \cdot C_X^i$$

$$r_2 = \eta_2 k_{v2} \cdot C_F^i$$

where the superindex i refers to the LS interface.

To prevent the degradation of F, it is proposed to conduct this reaction with simultaneous extraction of F into an organic solvent, where F does not longer react:

$$F(aq) \xrightarrow[k_{LL}a]{\textit{Extraction}} F(org)$$

These two processes (reaction + extraction) take place in a structured reactor like the one sketched in Figure 1. In this reactor, the acid catalyst is deposited as a washcoat layer on the surface of a foam structure. During operation the foam structure rotates very rapidly, allowing large interfacial contact between the aqueous and the organic phases, which behave as ideal well-mixed systems. Due to chemical affinity, the catalyst surface is fully wet by the aqueous solution, and does not have direct contact with the organic phase.

Assumptions:

- Although water is both a solvent and a reaction product, the volumetric flow and the holdup of the aqueous solution can be assumed constant.
- The organic and the aqueous solutions are completely immiscible.
- X and D are not soluble in the organic solvent.
- The catalyst layer may be considered as a flat slab.

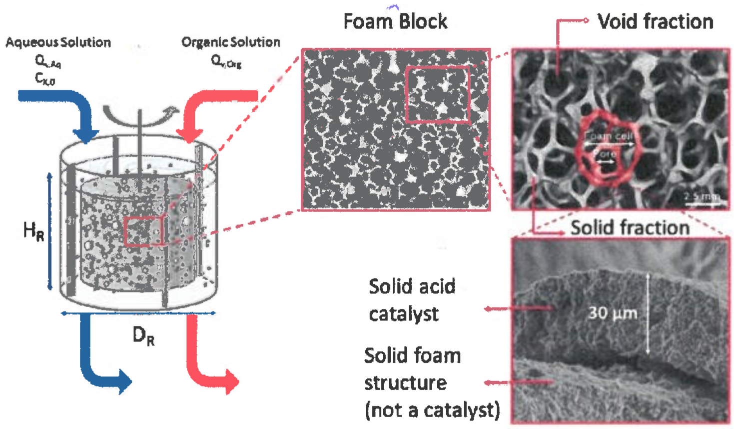

Figure 1: Sketch Structured Reactor

Data:
Height of the liquid in the reactor, H_R= 5 m
Diameter of the reactor, D_R= 0.5 m

Inlet concentration of X in the aqueous phase, C_X^{aq}: 300 mol/$m^3_{L,aq}$
Volumetric flow of aqueous solution, $Q_{v,aq}$=?? $m^3_{L,aq}$/s
Volumetric flow of organic solution, $Q_{v,org}$=?? $m^3_{L,org}$/s

Holdup aqueous phase, $\epsilon_{L,aq}$= 0.3 $m^3_{L,aq}/m^3_R$
Holdup organic phase, $\epsilon_{L,aq}$=0.6 $m^3_{L,org}/m^3_R$
Holdup solid phase, ϵ_S= ?? m^3_S/m^3_R

Catalyst holdup, ϵ_{cat}= 0.1 m^3_{cat}/m^3_S
Void fraction of foam block, ϵ_{void}= 0.8 $m^3_{[illegible]}/m^3_{foamblock}$ void
Washcoat thickness, d_{wc}: 30 μm

Kinetic constant at reaction temperature, k_{v1}= 1 $m^3_{L,aq}m^{-3}_{cat}s^{-1}$
Kinetic constant at reaction temperature, k_{v2}= 0.85 $m^3_{L,aq}m^{-3}_{cat}s^{-1}$

Effective diffusion coefficient in the porous layer, D_{eff}: $1{\cdot}10^{-10}$ m^2/s

Liquid-Solid mass transfer coefficient, k_{LS}: 1.0 $\cdot 10^{-4}$ $m^3_{L,aq}/\ m^2_i s$
Liquid-Liquid mass transfer coefficient, $k_{LL}a_{LL}$: 1.0 $\cdot 10^{-2}$ $m^3_{L,org}/\ m^3_R s$
Organic/Aqueous partition coefficient of F, m= 4 $m^3_{L,aq}/m^3_{L,org}$
Liquid-Solid interfacial area, a_{LS}=12.000 $m^2_i/m^3_{foamblock}$

Additional information:

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

$$\phi = \frac{1}{a_{cat}}\sqrt{k/D_{eff}}$$

where a_{cat} refers to the specific area of the catalyst in m_i^2/m_{cat}^3

Questions:

a) Derive the mole balances of X, F and D in all phases present in the reactor (1.5 points).

b) Calculate the total surface area that is available in this reactor for Liquid-Solid mass transfer (0.5 points).

c) Determine the rate limiting step in the conversion of X (1 point).

d) Calculate the volumetric flow rate that is needed to reach 80% conversion of X (1 point).

e) Propose 2 methods to increase the overall rate, and justify your answers (0.5 points).

f) Discuss the role of mass transfer in this process, and determine the value of $k_{LL}a_{LL}$ that is needed to ensure 95% selectivity of F (0.5 points).

Notes: In general, if in one of the sub-questions you cannot find the answer, you are encouraged to continue the exercise by making plausible assumptions. For example, in question c) you you may assume that the rate limiting step is the surface reaction rate (notice that this is not necessarily the correct answer).

Assignment 2: Reactor Selection & Optimization (5 points)

Part 2.1: Reactor Selection

The performance of a reactor is strongly determined by the residence time distribution (RTD) of the multiple phases present in the reactor. In particular, when the selectivity of a reaction is of concern, for example for a sequential reaction A $\rightarrow$ B$\rightarrow$ C in which B is the desired product, the RTD of the reactor will be a determining factor for the reactor selection.

Consider the following multiphase reactors:

i) A slurry bubble column
ii) A stirred tank batch reactor
iii) A monolith reactor
iv) A trickle bed reactor with 25% of stagnant liquid

Questions:

a) Sketch the E-curves as a function of the residence time for all phases (e.g., gas, liquid) and all reactors in the list above. Draw the E-curves of each reactor separately (1 point).

b) Rank the reactors for the highest selectivity to B for the liquid phase conversion of A $\rightarrow$ B$\rightarrow$ C. The reaction rate is limited by the intrinsic kinetics, which are described by a typical Langmuir-Hinshelwood kinetics model, and does not depend on the gas phase concentration. Calculations are not needed. Argument briefly why you pick this order (1 point).

c) For the same reaction described in b), rank the reactors for the highest selectivity to B when liquid-solid mass transfer limitations exist (1 point).

Part 2.2: Reactor Optimization

A heterogeneously catalyzed hydrogenation reaction is performed in a slurry bubble column for a liquid phase reactant with gas phase hydrogen. You are asked to double the production capacity of this reactor (more liquid feed). Assume that only hydrogen is limiting the rate (first order). The following options are available:

- A: Increase the temperature so that the intrinsic reaction rate doubles.
- B: Double the pressure at the same gas hold-up.
- C: Double the amount of catalyst.

- D: Increase the gas hold-up in the reactor, doubling a_{gl}.

Question:

d) Rank the most effective method for maintaining the desired conversion in the reactor (so A > B > C > D , C>A=B>D , or A=C>D > B etc) in case of the following cases:

1. Internal mass transfer limitations.
2. L-S external mass transfer limitations.
3. G-L mass transfer limited.

Motivate your answers as quantitative and concise as possible. Wrong arguments will costs you points, even when the final answer is correct. Answers without motivation are not graded (2 points).
