University of Pretoria
Department of Chemical Engineering
Reactor Design 410 - CRO410
Online Sick Test

Time = 180 minutes Full marks = 30

Scenario Description:

The first order catalysed gas phase reaction where: $\boldsymbol{A \rightarrow B + C}$ is allowed to take place in an ***adiabatically operated*** PACKED BED reactor where spherical, porous catalyst particles are used.

A feed stream that consists out of PURE gas A is fed to the reactor. The state variables of this stream at the inlet to the reactor are given in Table 1

Table 1 State of inlet gas stream that contains pure reactant A

Pressure (P_o)	1000	kPa
Temperature (T_o)	450	K
Volumetric flow rate (Q_o)	0.02	$m^3.s^{-1}$

Parameters relevant to the chemical reaction and components are given in Table 2

Table 2 Reaction rate and reaction energy parameters ($-r'_{A_i} = k'_o e^{-\frac{E}{RT}} C_A$)

Intrinsic pre-exponential rate constant (k'_o)	0.2936	$kg.m^{-3}.s^{-1}$
True activation energy (E)	31400	$J.mol^{-1}$
Heat capacity of A $\left(C_{p_A}\right)$	40	$J.mol^{-1}, K^{-1}$
Heat capacity of B $\left(C_{p_B}\right)$	25	$J.mol^{-1}.K^{-1}$
Heat capacity of C $\left(C_{p_C}\right)$	15	$J.mol^{-1}.K^{-1}$
ΔH_{RX} $\left(@T_{ref} = 298\ K\right)$	-20000	$J.mol^{-1}$

Some details on the porous catalyst are given in Table 3

Table 3 Some catalyst specific details

Effective diffusivity of A in catalyst pores (D_e)	7.5×10^{-8}	$m^2.s^{-1}$
Catalyst density (ρ_c)	1800	$kg.m^{-3}$
Bed porosity (ϵ)	0.4	-

The reactor is packed with $\boldsymbol{W = 110\ kg}$ of catalyst. In the following questions you will be required to evaluate the effect of catalyst particle size on the performance of the reactor by considering a particle size range $0.4\ mm \leq d_p\ 1\ mm$.

It is known that the Ergun constant for catalyst particles with $\boldsymbol{d_p = 1.0\ mm}$ is:

$\boldsymbol{K_{ERGUN} = 0.75 \frac{kPa}{kg}}$. Turbulent flow may be assumed.

1. Declare that the answers and code provided are your own work by answering the first true or false question.

2. What is the conversion of reactant A in a reactor with ***W = 110 kg*** of catalyst if the reactor is ***free*** of any internal or external mass transfer effects and catalyst particles with $\boldsymbol{d_p = 1\ mm}$ are used? *Give answer as a % and round to 3 significant numbers (i.e 12.3%)*

[5]

3. What is the conversion of reactant A in the same reactor if internal diffusion is considered? You may still assume that external diffusion effects are negligible. *Give answer as a % and round to 3 significant numbers (i.e 12.3%)*

[5]

4. The catalyst particle diameter is now reduced to $d_p = 0.5\ mm$. What is the conversion of A in the reactor with the new catalyst size? You may still assume external diffusion effects to be negligible and W = 110 kg. *Give answer as a % and round to 3 significant numbers (i.e 12.3%)*

[5]

5. In the particle range given in the problem scenario description above (i.e $0.4 \leq d_p \leq 1\ mm$, what is the optimum particle diameter that should be used in the reactor in order to maximise conversion of reactant A? (External diffusion effects negligible) *Give answer in units of mm and round to 3 significant numbers, i.e. 0.123 mm*

[8]

6. What is the conversion of the reactant at the given optimum particle diameter? *Give as % and round to 3 significant numbers i.e. 12.3%.*

[3]

7. Explain in a short paragraph why this optimum exists (type your answer in the space provided in Click-Up)

[4]

8. Upload your code as notebook file/s (no files no marks) in the ***sick test assignment*** tab that will be provided. Name the file/s: *surname_initials_stnumber_Q1.ipynb.* You can upload more than one file in this assignment. If you upload more than one file, ***please*** make use of descriptive file names (in addition to your surname).

Note that your test submission time will be compared with your notebook submission time in the assignment tab. ***NO MORE THAN 15 minutes*** *for assignment file upload. IF you experience trouble with Click-Up, email the notebook files as attachments (use the same naming protocol). Time of email will be considered in this case.* ***A 10% time penalty for every minute longer than 15 minutes between test and assignment submission will be applied***