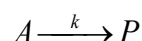


Module 5: Fast Reaction in the Different Ideal Reactors

Remark:

The following exercise was designed to show the effect of the choice of the reactor on the heat balance and on the process safety. Besides the quantitative aspects, a series of qualitative aspects of the performance of a reaction in the production scale should be discussed. For reasons of didactics, some assumptions were taken to simplify the calculations. The questions 1 to 4 may be treated independently.

Reaction:



The reaction is fast and follows a first order kinetics: $-\frac{dC_A}{dt} = k \cdot C_A$

At 50°C, the conversion reaches 99% in 60 s or $k = 0.077 \text{ s}^{-1}$.

Data:

$$C_A(t=0) = C_{A0} = 1000 \text{ mol/m}^3$$

$$\rho = 900 \text{ kg/m}^3$$

$$C_p = 2000 \text{ J/(kg.K)}$$

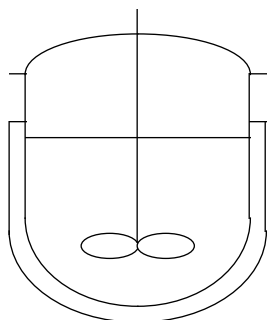
$$-\Delta H_r = 200 \text{ kJ/mol}$$

Question:

The performance of this reaction has to be studied in different types of reactor. For each reactor the heat balance and the reaction control will be discussed. Further the thermal aspects of a 100 times slower reaction will be considered. The reactors are :

- Batch reactor
- Semi-batch reactor
- Tubular reactor (plug flow)
- Continuous stirred tank reactor

1 Batch Reactor

**Data :**

Volume of reaction mass: 5 m³

Initial temperature: 50°C

Heat exchange area: 15 m² (i.e. 3 m²/m³)

Overall heat transfer coefficient: 500 W/(m².K)

Temperature difference: $T_r - T_c = \text{constant} = 50^\circ\text{C}$
(Simplification)

1.1 Adiabatic Reaction

- adiabatic temperature rise ?
- under which conditions can this reaction be performed under adiabatic conditions?

1.2 Isothermal reaction

- can this reaction be performed under isothermal conditions ?
- compare the heat balance of the adiabatic reaction (question 1.1) with the isothermal
- compare the heat balance in production scale with the same reaction performed in a 0.5 litre laboratory flask with a heat exchange area of 0.04 m².

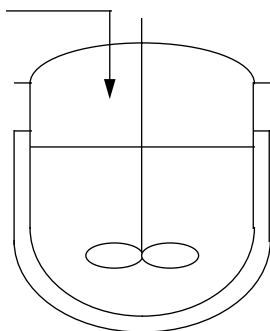
1.3 Cooling failure

What happens in case of cooling failure in case 1.1 and 1.2. ?

1.4 Slow Reaction

What happens if the reaction is slower by a factor of 100 ?

2 Semi-Batch Reaction



The compound A is fed as a concentrate solution to a reactor containing an inert solvent.

Initial temperature: 50°C

Volume (assumed to remain constant) : 5 m³

Heat exchange area: 15 m² (i.e. 3 m²/m³)

Overall heat transfer coefficient: 500 W/(m².K)

Temperature difference: $T_r - T_c = \text{constant} = 50^\circ\text{C}$
(Simplification)

2.1 Isothermal reaction

Which feed time is required to assure isothermal conditions at 50°C ?

2.2 Slow reaction

What happens with a slow reaction ?

2.3 Cooling failure

What happens in case of cooling failure ?

3 Tubular Reactor



3.1 Reactor design

Calculate the dimensions of the reactor in order to achieve the same performance as the 5 m³ semi-batch reactor with a time cycle of 2 hr's. Pure plug flow with a flow rate of 1 m/s will be assumed.

The overall heat transfer coefficient is 1000 W/(m²·K).

Why is its value larger than in the stirred tank ?

3.2 Isothermal reaction

Under which conditions is this regime possible ?

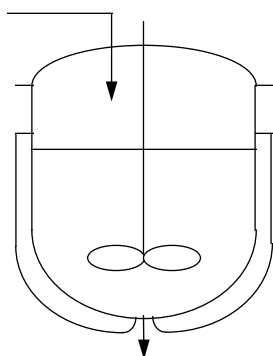
3.3 Slow reaction

What happens with a 100 times slower reaction ?

3.4 Cooling failure

What happens in case of cooling failure ?

4 Continuous Stirred Tank Reactor



Normalised jacketed reactors:

V (m ³)	0.63	1.0	1.6	2.5
A (m ²)	2.82	4.2	6.6	8.9

4.1 Reactor design

What must be the volume of the CSTR in order to achieve the same performance as the 5 m³ semi-batch reactor with time cycle of 2 hr's with a conversion of 99% ?

4.2 Isothermal reaction

Under which conditions is this strategy possible ?

4.3 Slow reaction

What happens with a 100 times slower reaction ?

4.4 Cooling failure

What happens in case of cooling failure ?