Solution Module 5: "Fast Reaction in the Different Ideal Reactors"

1 Batch reactor

1.1 Adiabatic reaction

Under adiabatic conditions, no heat exchange occurs. Therefore the heat produced by the reaction is transformed into a temperature rise:

For a conversion of 100 %, the adiabatic temperature rise is:

$$\Delta T_{ad} = \frac{C_{A0} \cdot (-\Delta H_R)}{\rho \cdot Cp} = \frac{1000 mol/m^3 \times 200 kJ/mol}{900 kg/m^3 \times 2 kJ/(kg \cdot K)} = 111 K$$

With an initial temperature of 50°C, the temperature will reach 161°C at the end of the reaction. If no secondary reaction is triggered at this temperature, and if no pressure rise occurs, this reaction is theoretically possible. The problem is due to mechanical stress in the reactor wall due to the fast temperature changes.

1.2 Isothermal reaction

An overall heat balance gives:

Heat production: Qrx = V. CA_0 (-ΔHr) = 5 m^3 x 1000 mol/m^3 x 200 kJ/mol = 10^6 kJ

Heat removal: qex = U . A . ΔT = 500 W/(m^2.K) x 15 m^2 x 50 K = 375 kW

Since the conversion is 99 % in 1 minute, the heat which can be removed is:

Qex = qex . t = 375 kW x 60 s = 22500 kJ

Thus only ca. 2% of the heat produced by the reaction can be removed by the heat exchange system. Thus the reactor behaves quasi adiabatic. In other words, the reaction is so fast that the heat exchange system is not able to remove any significant heat.

In the laboratory scale a similar heat balance is:

Heat production : 100 kJ and heat removal: 60 kJ

At this scale, 60% of the reaction heat can be removed. This shows the importance of the heat balance in scale up considerations.

1.3 Cooling failure

Since the heat exchange is so small compared to the heat production, the cooling failure plays no significant role.

1.4 Slow reaction

For a 100 times slower reaction (k= 0.00077 s^{-1}) the adiabatic temperature rise will be the same. But taking the acceleration of the reaction with temperature into account, the reaction time will be acceptable:

The initial heat release rate is :

q_0 = k.CA_0.(-ΔHr)/ρ = 0.00077 x 1000 x 200000 / 900 = 171 W/kg

The reaction time can be estimated by:

$$TMR_{ad} = \frac{Cp \cdot R \cdot T^2}{q_0 \cdot E} = \frac{2000 \times 8.314 \times 323^2}{171 \times 100'000} \cong 100 s$$

For isothermal conditions, the overall balance gives a heat removal of 2.25 . 10^6 kJ which is more than 2 times the heat production. This consideration is erroneous. For a first order reaction, where the maximum heat release rate takes place at the beginning and decreases exponentially with time, the differential form of the heat balance must be used:

$q_0 = k.CA_0.V.(-\Delta Hr) = 0.00077 \times 1000 \times 5 \times 200$ kW = 770 kW

qex = 373 kW

To ensure a good control of the reaction it must be started at a lower temperature perhaps under adiabatic conditions, followed by a period with maximal cooling when the desired temperature level is reached. Therefore, batch reactions are often performed in the so called polytropic mode of operation.

2 Semi-batch Reaction

2.1 Isothermal reaction

From 1.2: qex = 375 kW

For a fast reaction, the feed rate can be adapted in such a way to give the heat exchange system enough time to remove the heat of reaction:

$$q_{RX} = \frac{V \cdot C_{A0} \cdot \left(-\Delta H_R\right)}{t_{feed}} = \frac{Q_{RX}}{t_{feed}} = q_{EX}$$

Thus : $t_{feed} = \frac{Q_{RX}}{q_{EX}} = \frac{10^6 kJ}{375 kW} = 2667 s \cong 45 \min$

2.2 Slow reaction

From the point of view of the heat balance, the feed time could be the same than above. Nevertheless for slow reaction, the accumulation will require a slower addition.

2.3 Cooling failure

For the fast reaction, if the feed is immediately stopped after a cooling failure has occurred, the reactor reaches a safe state.

For the slow reaction, the behaviour will result from the accumulation of non converted reactants. The temperature increase could trigger secondary reactions.

3 Tubular Reactor

3.1 Reactor design

The semi-batch reactor produces 5 m^3 of product solution every 2 hr's. Therefore, in a continuous reactor, the flow rate must be 2.5 m^3/hr or $6.94 \cdot 10^{-4}$ m^3/s. In order to achieve a space time $\tau = 1$ minute, necessary to reach a conversion of 99%, the volume is:

$$V = \tau \cdot \dot{v}_0 = 0.042 m^3$$

With a flow rate of 1 m/s, the length is 60 m.

Hence the diameter is : $d = \sqrt{\frac{4V}{\pi}} \cong 0.03\ m$

The increase of the heat transfer coefficient is due to a higher turbulence at the wall compared to a stirred tank.

3.2 Isothermal reaction

The overall heat balance gives:

Heat production:

$q_{rx} = \dot{v}_0 \cdot C_{A0} \cdot (-\Delta H_R)$ = $6.94.10^{-4}$ m^3/s x 1000 mol/m^3 x 200 kJ/mol = 139 kW

Heat exchange area: $A = \pi.d.L = 3.10^{-2}$ m x 3.14 x 60 m = 5.65 m^2

Heat removal: $q_{ex} = U . A . \Delta T$ = 1kW/(m^2.K) x 5.65 m^2 x 50 K = 283 kW

The overall balance seems to allow cooling. This is due to a more favourable ratio area / volume. Nevertheless, similar to batch reactors where the heat release rate changes with time, in the plug flow reactor, the heat release rate will change along the reactor. The maximum is located at the entrance of the tube. A more accurate balance established for the portion where the first 10 % of the conversion are obtained, shows that 6.5 kW can be eliminated whereas 13.9 kW are produced. Thus a hot spot will develop at the beginning of the reactor. This can be eliminated by establishing an increasing temperature profile in the reactor, as an example by starting at a lower temperature. This solution will require an increase of the reactor length.

3.3 Slow reaction

A 100 times slower reaction will lead to an unrealistic reactor length of 6 km! But no hot spot will be observed. Continuous reactors are unsuited for slow reactions.

3.4 Cooling failure

The situation is most critical at the entrance of the reactor where the reaction will continue under quasi adiabatic conditions, even if the feed has been stopped. The temperature increase can be limited by an adequate construction: increase of the heat capacity of the reactor itself.

4 Continuous Stirred Tank Reactor

4.1 Reactor design

The mass balance is: $\tau = \frac{V}{\dot{v}_0} = \frac{C_{A0} \cdot X_A}{-r_A}$

For a first order reaction: $-r_A = k \cdot C_{A0} \cdot (1-X_A)$

Hence: $\tau = \frac{X_A}{k \cdot (1-X_A)} = \frac{0.99}{0.077 \times 0.01} = 1286 s$

The reactor volume is : $V = \tau \cdot \dot{v}_0 = 1286\ s \times 6.94.10^{-4}\ m^3/s = 0.9\ m^3$

The reactor of 1 m^3 is best suited. The heat exchange area is: $A = 4.2\ m^2$.

4.2 Isothermal reaction

Heat balance:

Heat production:

$q_{rx} = \dot{v}_0 \cdot C_{A0} \cdot (-\Delta H_R) = 6.94.10^{-4}\ m^3/s \times 1000\ mol/m^3 \times 200\ kJ/mol = 139\ kW$

Heat exchange : $q_{ex} = U \cdot A \cdot \Delta T = 0.5\ kW/(m^2.K) \times 4.2\ m^2 \times 50\ K = 105\ kW$

The difference of 34 kW which cannot be eliminated by the jacket, can be eliminated by using the cooling effect of the feed:

$$\frac{q_{RX} - q_{EX}}{\dot{v}_0 \cdot \rho \cdot Cp} = \frac{139 kW - 105 kW}{6.94 \cdot 10^{-4} m^3/s \times 900 kg/m^3 \times 2 kJ/(kg.K)} \approx 27 K$$

Thus a feed temperature of 23 °C will allow to maintain a reactor temperature of 50°C.

4.3 Slow reaction

For a 100 times slower reaction, the heat exchange becomes fully uncritical. But the conversion of 99% can only be reached with a volume of 90 m^3, which is unrealistic. The situation becomes better with a higher reactor temperature or with a different combination of reactors: cascade of CSTR's or CSTR followed by a tubular reactor.

4.4 Cooling failure

If the feed is immediatly stopped in case of malfunction, the CSTR is uncritical: the non converted reactant is only 1%, resulting in a ?Tad of ca. 1°C