Answers to exercise

Substitution reaction in semi-batch reactor (DSC)

Question 1

The energy potential or the heat per unit mass is:

$Q'_{dc} = 1150\ kJ\ kg^{-1}$.

The specific heat capacity is $c'_P = 1.7\ kJ\ kg^{-1}\ K^{-1}$

The adiabatic temperature rise is then $\Delta T_{ad} = \frac{Q'_{dc}}{c'_P} \approx 677\ K$

Such high a temperature rise corresponds to a *high severity*. Thus it is important to assess the triggering probability.

Question 2

The energy potential of the main reaction is:

$Q'_{rx} = 300\ kJ\ kg^{-1}$.

The specific heat capacity is $c'_P = 1.7\ kJ\ kg^{-1}\ K^{-1}$

The adiabatic temperature rise is then $\Delta T_{ad} = \frac{Q'_{rx}}{c'_P} \approx 176\ K$

Such a temperature rise corresponds to a *medium severity*.

Assuming 100% reactant accumulation (as in a batch reactor), the theoretically achievable temperature would be: $T_{max,th} = T_P + \Delta T_{ad} = 80 + 176 = 256\ °C$

Even with a lower degree of accumulation it cannot be excluded that in case of loss of control of the reaction, the decomposition could be triggered. In such case, the final temperature would be:

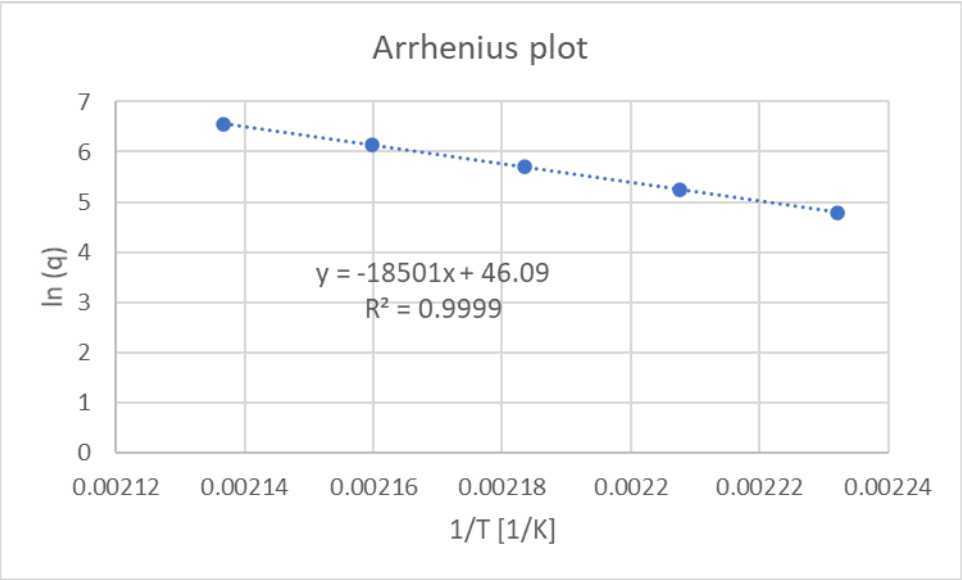
$T_f = T_p + \Delta T_{ad,rx} + \Delta T_{ad,dc} = 80 + 176 + 677 = 933°C$

Question 3

The thermal signal is uniformly decreasing: this corresponds to a nth order reaction, i.e. the decomposition id not autocatalytic.

To determine TMRad, the Activation energy is calculated based on an Arrhenius plot:

Temperature (°C)	Maximum heat release rate (W/kg)	T (K)	ln q
175	120	448	4.79
180	190	453	5.25
185	300	458	5.70
190	460	463	6.13
195	700	468	6.55



The activation energy is 153.8 kJ/mol.
The TMRad are

Temperature (°C)	Maximum heat release rate (W/kg)	TMRad (h)
100	0.03	119
105	0.06	63
110	0.11	34
115	0.2	19
120	0.37	11
125	0.67	6
130	1.2	3.5

The time to maximum rate is 24 hours at 113°C and 8 hours at 122°C. The probability of the runaway of the decomposition reaction is low below 115°C and high above 125°C.