

Module 4 Solution: “Interpretation of a DSC”

Decomposition of a reaction mass

- **What are the different curves on the figure?**

The blue and black curves are the decomposition of the reaction mass. The measurement was performed on two samples. The red curve is the 2nd heating for one of the two measurements. It is thus the measurement of the decomposed material. This curve is used as a help to set the baseline.

- **What is the severity of the decomposition?**

The decomposition energy is between 694 and 709 kJ/kg. With a c_p of 2 kJ/(kg·K), the ΔT_{ad} is around 350 K. The severity is thus high

- **Is a batch distillation temperature of 140°C safe?**

To determine whether a batch distillation is safe, the TMR_{ad} at 140°C has to be determined.

Applying the rule of thumb:

$$q'_{(T)} = q'_{(T_{ref})} \times \exp \left[\frac{-E_a}{R} \times \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad TMR_{ad}(T) = \frac{c'_p R T^2}{q'_{(T)} E_a}$$

From the thermogram, the left limit of the peak is 218°C.

$$T_{ref} = 218^\circ\text{C} = 491\text{K}$$

$$q'_{ref} = 20 \text{ W/kg}$$

$$E_a = 50'000 \text{ J/mol}$$

$$T_p = 140^\circ\text{C} = 413\text{K}$$

$$q'_{(140^\circ\text{C})} = 20 \times \exp \left[\frac{-50'000}{8.314} \times \left(\frac{1}{413} - \frac{1}{491} \right) \right] = 1.98 \text{ W/kg}$$

$$TMR_{ad}(T) = \frac{c'_p R T^2}{q'_{(T)} E_a} = \frac{2000 \cdot 8.314 \cdot 413^2}{1.98 \cdot 50'000} = 28'666\text{s} = 8\text{h}$$

- **What is the thermal risk?**

The thermal risk is high: high severity and medium to high probability of triggering the decomposition reaction.

By varying the temperature, one finds that the T_{D24} (T for which the TMR_{ad} is 24h) is 107°C.