

# DSC evaluation

This software option provides you with a number of DSC-specific evaluation tools for both quality

control and research and development purposes. The easy-to-use routines allow important characteristic values to be obtained immediately without the need for time-consuming manual calculations.

The software option includes the following evaluation routines:

- **Content**  $G = \Delta H / \Delta H_{Lit} \cdot 100 \%$
- **Crystallinity**  $K = \Delta H / \Delta H_{100\%} \cdot 100 \%$
- **Conversion**  $\alpha = \Delta H_{part} / \Delta H_{tot} \cdot 100 \%$
- **Enthalpy**  $H = \int \frac{dH}{dt} dt$
- **Glass transition** (with or without the relaxation peak)

( $\Delta H_{Lit}$  = literature value,  $\Delta H_{100\%}$  = heat of fusion of the 100% crystalline material,  $H_{part}$  = partial integral and  $\Delta H_{tot}$  = measured total integral).

The content routine allows the proportion of a component in a substance to be determined. It is assumed that the effect used for the evaluation occurs in isolation and that the enthalpy change for the pure component is known ( $\Delta H_{Lit}$ ).

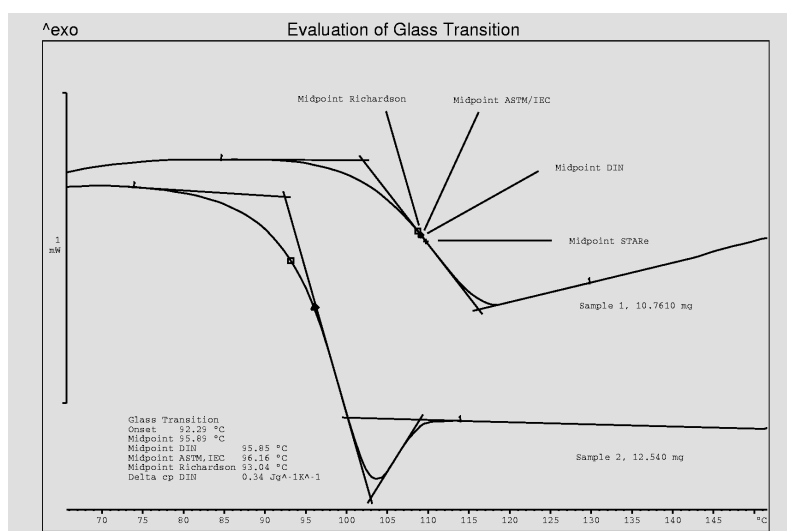
The crystallinity is a characteristic value that is used to characterize polymers. The ratio of the measured heat of fusion to the literature value for the 100% crystalline substance is calculated. The calculation of the conversion curve is the basis for the evaluation of the kinetics of isothermal and dynamic reactions (curing, decomposition). The determination of the liquid fraction of fats or oils is also based on this evaluation. Cases in which a sample has already partially reacted ( $\alpha_{start} > 0\%$ ) or in which a reaction does not go to completion ( $\alpha_{end} < 100\%$ ) can also be taken into account.

The enthalpy program allows the enthalpy temperature function of a substance to be calculated. The glass transition can be calculated both with and without the relaxation peak according to several different standards. Since the glass transition extends over a temperature range, several different values are determined in the evaluation. These are defined differently in the various standards so that the evaluation method has an influence on the result. A number of

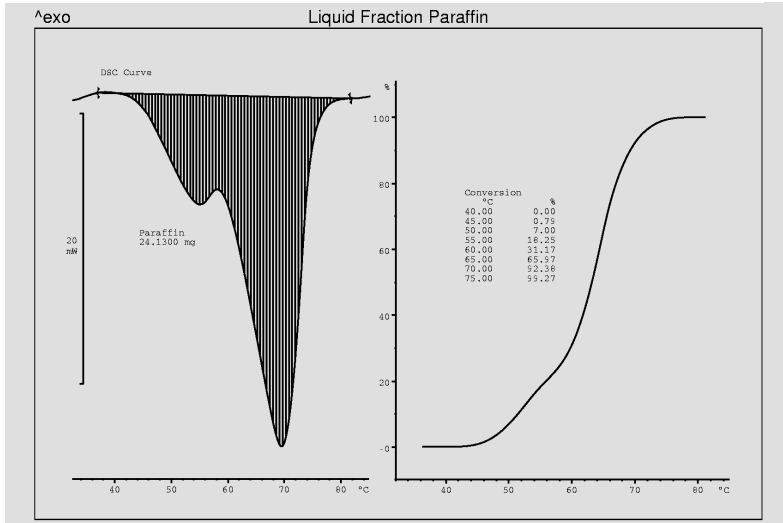
standards (DIN, ASTM/IEC etc.) are supported in this option so that you can choose which one you use for the evaluation:

- STAR<sup>e</sup>:** Point of intersection of the DSC curve and the bisector of the angle formed by the extrapolation of the baselines before and after the transition
- ASTM/IEC:** Midpoint of the segment of the inflectional tangent between the onset and endpoint
- Richardson:** Point of intersection of the enthalpy temperature function according to Richardson
- DIN 51007:** Midpoint of the segment of the mid-tangent between the extrapolated baselines

The glass transition of two epoxy resins (with and without relaxation) after curing at 140 °C, evaluated according to different methods.

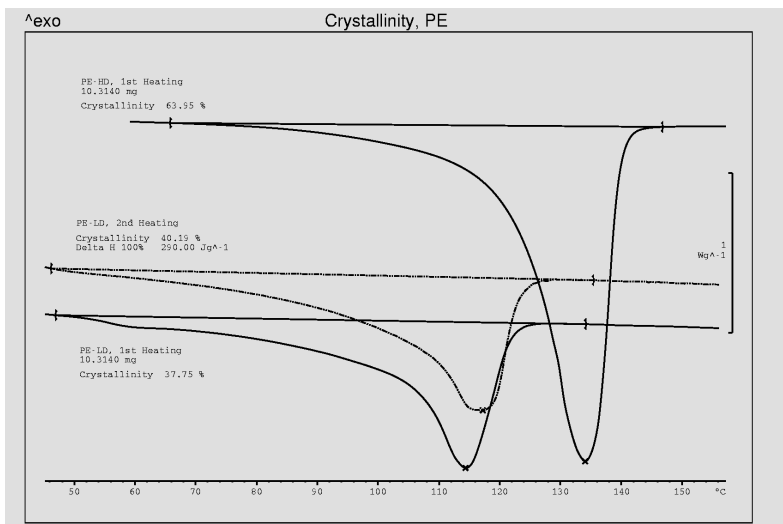


## Application examples



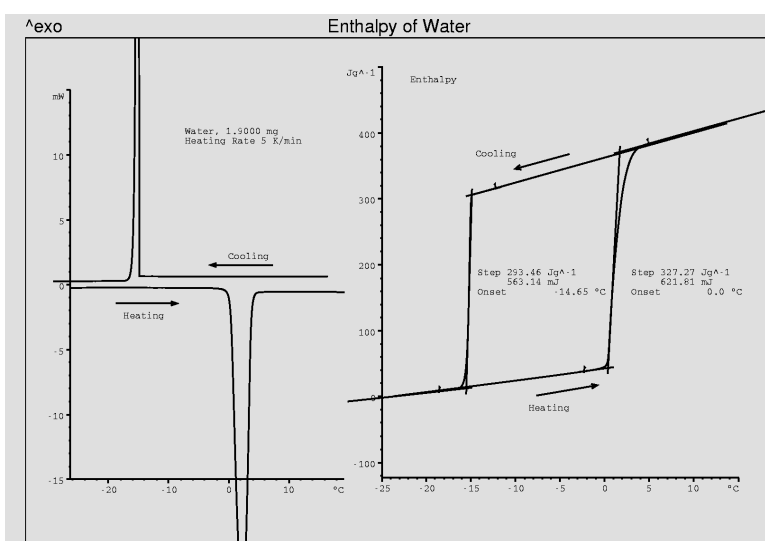
### Liquid fraction

The conversion curve is the best means of characterizing substances that melt over a wide temperature range. In connection with fats and waxes the terms liquid fraction or molten fraction are also used. This indicates the percentage of the substance that has already melted at any given temperature. Using the DSC melting curve of paraffin as an example, the liquid fraction is calculated from the conversion curve and the results shown in tabular form. At 65 °C for example 66% of the paraffin has melted.



### Crystallinity

The example shows the DSC curves of different samples of polyethylene. The crystallinity is calculated as the ratio of the measured heat of fusion of the sample to that of 100% crystalline PE (which is assumed to be 290 J/g, literature value). The crystallinity of the polyethylene PE-HD and PE-LD samples used in this example are clearly different. A second measurement (PE-LD, 2nd heating run) of the same sample is often performed in order to eliminate the effects of thermal history. This data is then used for the calculation. It is quite possible that the two DSC curves differ to a certain extent, which in turn affects the value calculated for the crystallinity (see PE-LD 1st/2nd heating runs).



### Enthalpy temperature function

The calculation of the enthalpy curve is shown using the crystallization and melting of water as an example. The DSC heating and cooling runs (both blank curve corrected) are shown in the left part of the diagram. As a result of supercooling the crystallization of the water occurs at -14.6 °C, the melting however as expected at 0 °C. In the right part of the diagram the enthalpy curve is shown as a function of the reference temperature for both processes (the ordinate scale is arbitrarily chosen). The enthalpy steps correspond to the heat of fusion and the heat of crystallization of the water. Whereas the value of 327.3 J/g for the heat of fusion at 0 °C corresponds quite well with the literature value, the value of 293.5 J/g for the heat of crystallization at -14.6 °C is distinctly lower. This effect is caused by the different slope of the enthalpy temperature function of ice and of water (the slope is equal to the specific heat capacity).