Mathematics

This option offers you a number of useful evaluation routines that can be applied to all curves. Besides the purely mathematical functions such as integration, derivative or curve averaging you have a tool that allows you to present curves and evaluations in your own desired formats. This could be for smoothing curves, separating segments of curves or selecting regions of curves.
The functions include:

Reporting: (Layout)	**Cut to frame**	Select the region of the curve, if only the effect is to be shown.
	Smooth	Smoothing of curves (to eliminate noise)
	Take apart	Dividing the curve into temperature segments
Averaging:	**Add curves**	Averaging of several measurements
	Divide/Multiply	Division and multiplication with a factor and/or a unit (conversion to another physical unit)
Curve subtraction:	**Subtract curves**	Subsequent blank correction, if the automatic correction was not applied in the measurement
Periodic signals:	**Envelope**	Calculation of the upper and lower envelopes of a periodic signal
Peak separation:	**1st derivative**	Calculation of the slope of a curve (very useful for distinguishing between individual weight loss steps in TGA measurements)
Special features:	**Subtract line**	Simple drift correction (straight line subtraction)
	Subtract poly-line	Draw and subtract a manually created base-line (polygonal line, formed graphically from individual straight lines)
	Integral	Calculation of the integral curve (without baseline selection)
	Integration	Integration of the ordinate above the abscissa. Important mainly for peak area determinations (e.g. imported MS measure-ments) or for the calculation of the heat of transformation from a cp temperature function.
	2nd derivative	Calculation of the rate of change
	Divide curves/ Multiply curves	Division and multiplication of two curves (e.g. division by the heating rate)

The calculation of the derivatives and of the smoothing of curves is based on a compensation function that is applied to a region of a curve (window) with a choice of the number of data points and of the order of the polynomial.

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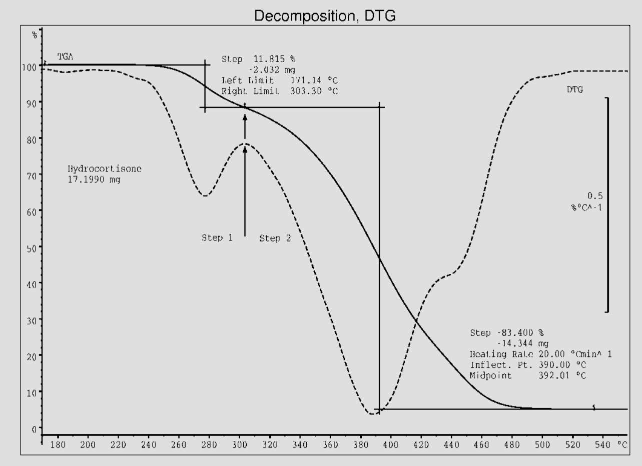
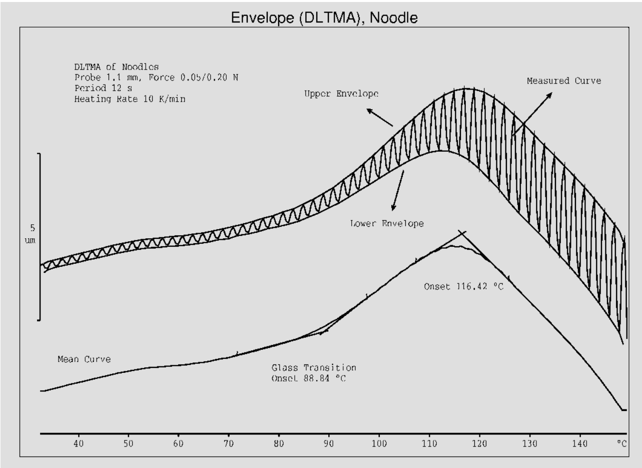
Application examples



Decomposition of a pharmaceutical active ingredient

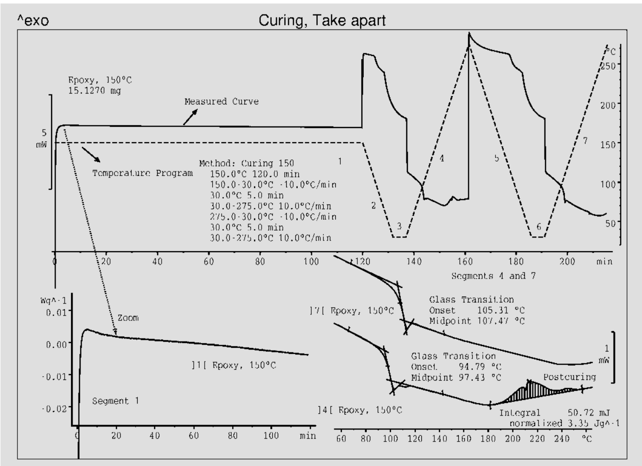
The example shows the thermogravimetric analysis of the decomposition of hydrocortisone, a pharmaceutical active ingredient, which decomposes in several steps. If the steps overlap, as in this case at about 310 °C, then an exact determination of the evaluation limits and hence the weight loss for each individual reaction step is difficult using the original curve. In such a case the calculation of the 1st derivative (DTG curve, shown here already smoothed) is very helpful. It shows clearly the transition of the two steps (maximum between two negative peaks) and allows a unambiguous evaluation, since the beginning and the end of the individual decomposition steps can be defined. In this example the transition of the two steps is at about 303.3 °C and the weight loss of the first step 11.82%.



Glass transition of noodles

DSC is often at the limit of its sensitivity when determining glass transitions of low intensity. In such cases it is preferable to use dynamic load TMA (DLTMA). The example shows such a measurement of a noodle, whose glass transition temperature is to be determined.

The upper part of the diagram shows the measured curve with the upper and lower envelopes. The mean curve is calculated by adding the two curves and dividing by two. From this it is evident that the sample expands up to about 110 °C and afterwards undergoes plastic deformation. The change of slope at 88.8 °C is considered to be caused by the glass transition. The amplitude of the DLTMA curve is determined by subtraction of the envelopes and division by two. It represents elastic deformability.



Curing of epoxy resins

Both the degree of curing and the glass transition temperature Tg of the cured epoxy are of interest in the investigation of the isothermal curing of epoxy resins (e.g. powder coatings). This information can be obtained from a single DSC experiment: after curing isothermally for 120 minutes at 150 °C the sample is cooled down to 30 °C under controlled conditions, held isothermally for a short time and then heated twice dynamically up to 275 °C. In the upper part of the diagram the method and the temperature program as well as the curves measured with respect to time are shown (the numer next to the curve indicates the particular segment). The segments of interest for the evaluation are selected with the function 'take apart'. These include the actual isothermal curing (segment 1) and also both the dynamic heating segments 4 and 7. For the latter two, only the temperature region between 55 °C and 265 °C is shown (function 'cut to frame').

The 1st segment allows the determination of the reaction enthalpy and is the basis for the conversion calculations and kinetic evaluations. It can be seen from the expanded curve (zoom) that even after 120 minutes the curing reaction is not complete. The consequences of this incomplete curing at 150 °C are a glass transition temperature Tg that is too low and a post-curing reaction in segment 4. The degree of curing and therefore the Tg (segment 7, further heating run) satisfy the requirements only after this post-curing step.

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