Order Form (DSC Curve Solutions®)

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Goods: DSC Curve Solutions® v3.0 (DSC curve analysis and simulation software)
Supplier: J & C Consultation and Technology (Vic reg. no: B2022626B) ABN: 78279830190
6 Barter Crescent, Forest Hill, Vic 3131, **Australia**

Price:
free for 3 day trial license;
AUD$30 for single 1 month license (once only)
AUD$200 for single 3 month license
AUD$600 for single 12 month license
AUD$1,600 for single perpetual license
AUD$2,980 for 3 perpetual licenses
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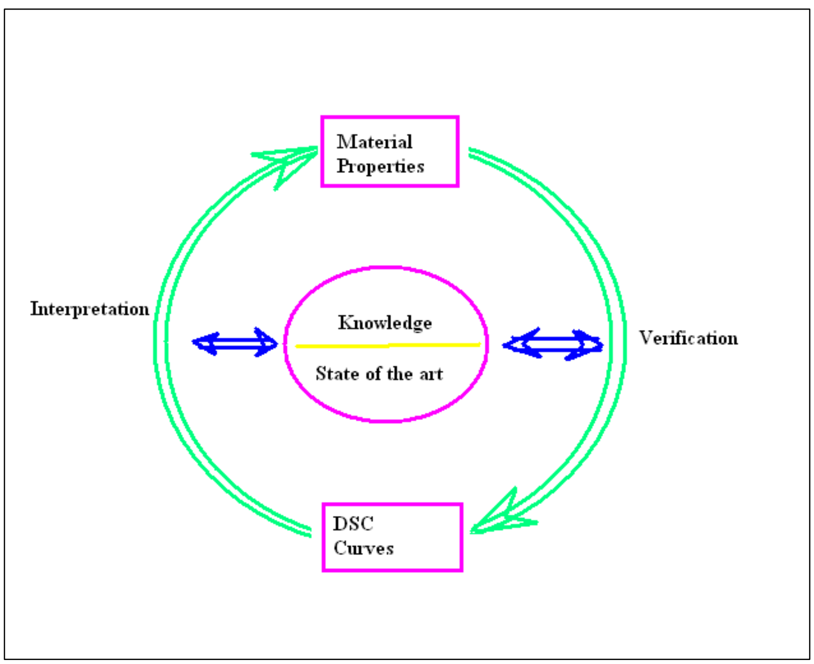
DSC Curve Solutions® (DCS)

— The world's first, the world's only —

Software DSC Curve Solutions® (DCS) represents a novel approach for thermal analysis that allows one to simulate full DSC curves vividly for experiments under any conditions for a range of thermal events; so that you can extract **all the relevant sample properties from any single DSC run**.

How can DCS be useful?

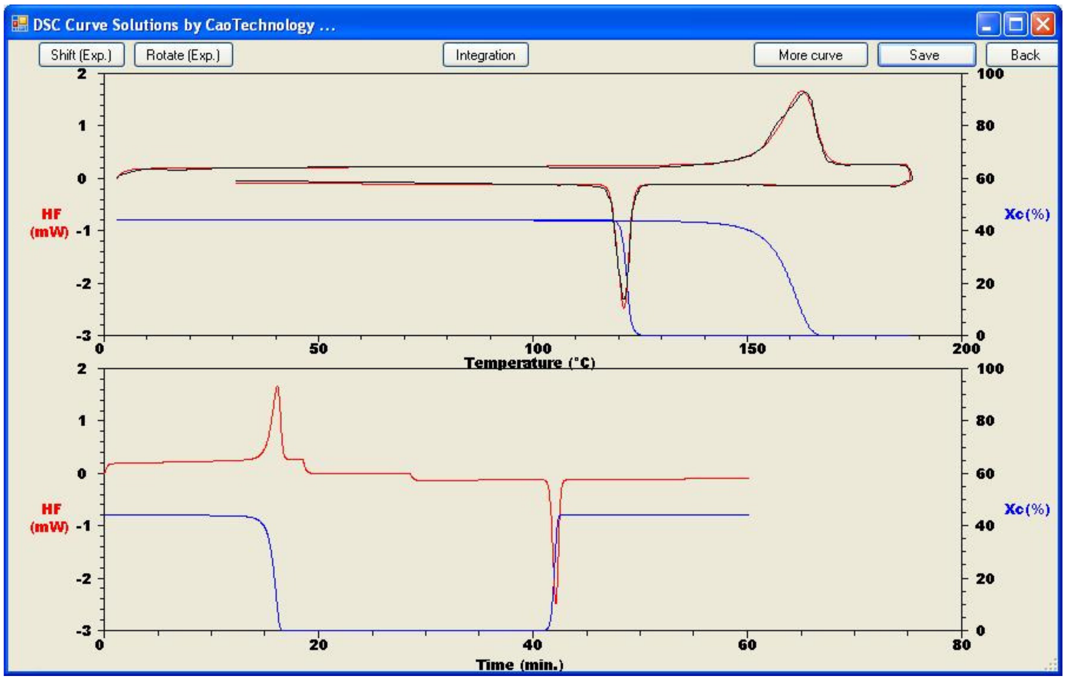
- It obtains sample thermal properties by fitting DSC curve with DCS curve - interpretation and verification, fused as one;
- It extracts more thermal properties than any conventional DSC analysis methods do; e.g. determine curing/crystallisation kinetics from a single non-isothermal DSC run;
- It covers a range of thermal events *i.e.* heat capacity, glass transition, enthalpy relaxation, melting and crystallisation, curing and reactions; furthermore its multi-component function allows you to deconvolute complicated DSC curves readily;
- It resolves your headache when observing a "shifting" "baseline" before and after a thermal event. DCS tells you why the "baseline" "shifts" and how to fit the "baseline".
- … …



- It covers DSC runs under any experimental conditions e.g. linear heating, sinusoidal (one or more freq.) and/or saw-tooth modulation if wished;
- It is a perfect aid to learn and teach DSC and polymers – you'll have a better understanding of the both.
- No training, no tutorial and no help is needed, you'll be an instant expert of DCS.

Examples of DCS applications

An iPP sample was heated from 5°C to 185°C at 10°C /min, stayed isothermally for 10 min, followed by a cooling at 5°C/min to 30°C, with its DSC experimental curve being shown in the black line in the figure below (digitised from Fig.2, Cao and Sbarski, *Polymer* **47**, 27-31(2006)). Now, simply key in all these known experimental conditions into DCS, we obtain simulated DSC curves shown in the red line. After several trial-and-error tuning reiterations, we fit the DSC curve with DCS curve to our satisfaction, leading to determination of following parameters from just a single DSC run:



Specific heat capacity, c_p = 1.10 J/Kg at 0°C, ramping linearly towards 1.66 J/Kg at 200°C;

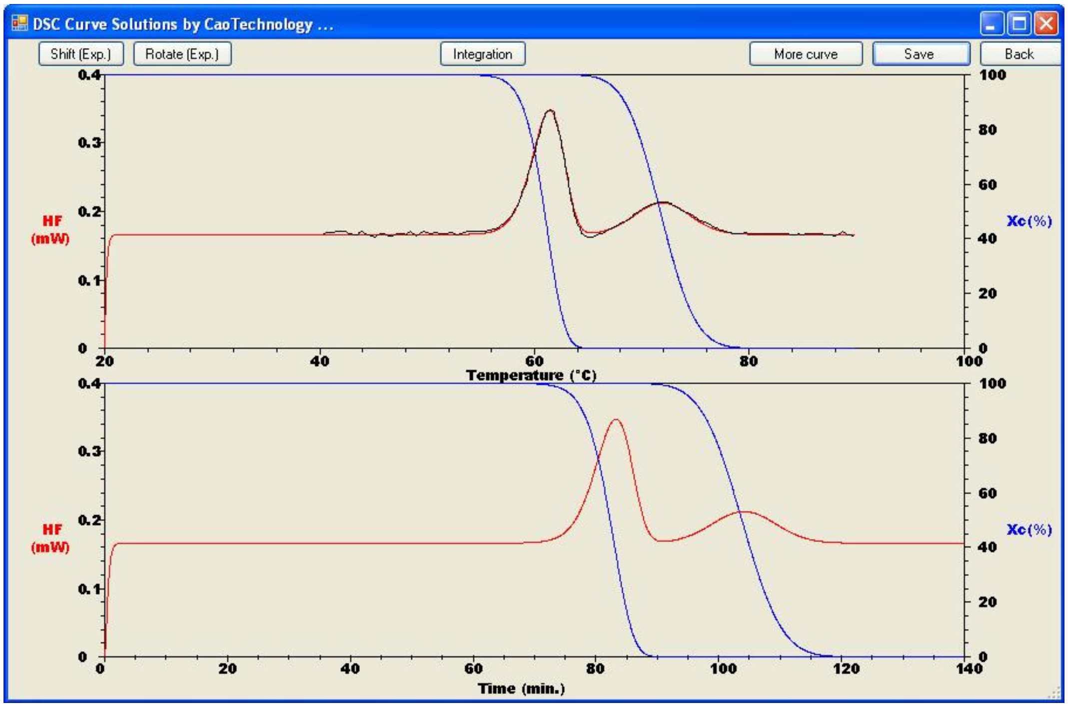
Melting enthalpy, ΔH = 95.2 J/g,
Melting peak temperature, T_m = 161.5°C,
Half width of the Gaussian crystallite size distribution, μ_m^2 = 65,
with its asymmetric factor of the Gaussian crystallite size distribution = -0.06,

Crystallisation rate factor, A_k = 0.024,
Maximum crystallisation rate temperature T_{max} = 118.5°C;
Half width of the crystallisation rate distribution, μ_k^2 = 120,
and Avrami index, n = 4.

Given that the melting enthalpy for 100% crystallised iPP is 207 J/g,
we obtain the crystallinity curve as well (the blue curves)

Just from a single DSC run, we have fully determined all the relevant properties, in particular, the melting and crystallisation properties of the sample.

DSC curve deconvolution



Experimental DSC curve for a multi-domain immunoglobulin G (IgG) protein shows two denaturasation (melting) endotherms slightly overlapping (curve in black); this is compared with the theoretical curve simulated using DCS v3.0. They are fitting very well. The DSC curve is readily deconvoluted and following parameters are obtained:

Domain 1: denaturation enthalpy, ΔH = 12.5 J/g;
peak temperature, Tm = 61.2°C,
half width of the Gaussian distribution, mm2 = 12;
asymmetric factor of the Gaussian distribution = -0.065,

Domain 2: denaturation enthalpy, ΔH = 5.4 J/g;
peak temperature, Tm = 71.7°C;
half width of the Gaussian distribution, mm2 = 37;
asymmetric factor of the Gaussian distribution = 0.

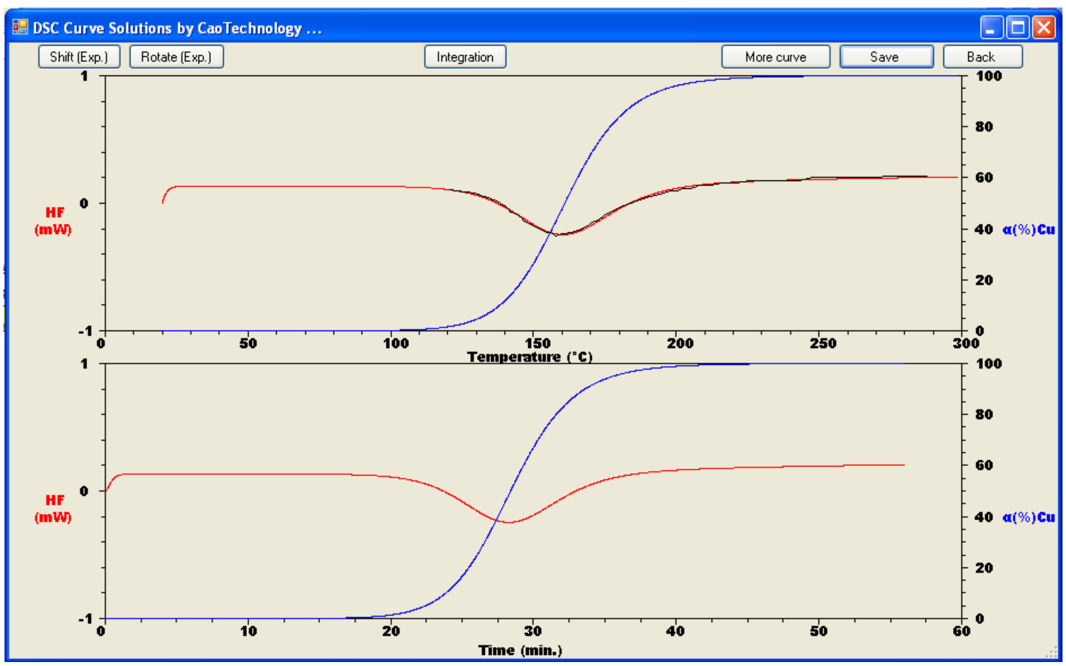
Non-isothermal kinetics and DCS

We need to know not only the activation energy, Ea, and pre-exponential factor, A, but also all the relevant parameters as well as the reaction model so that we can calculate the degree of reaction for any given thermal history - the usefulness of a methodology lies in its predictive power !

With DSC Curve Solutions® (DCS), one can determine all the kinetic parameters from any single DSC run for any given model.

Example of non-isothermal epoxy curing

Following example shows how DCS can be employed to study non-isothermal curing kinetics for epoxy resins. The black curve in the figure below is the exotherm of a DSC run at 5°C/min for an epoxy resin. Using the autocatalytic model shown below, we determine the kinetic parameters of the epoxy resin by simply fitting this single run DSC curve (black) with DCS curve (red) to satisfaction:



Autocatalytic model: $$\frac{d\alpha}{dt} = \left[k_{10} \exp\left(-\frac{E_{a1}}{RT}\right) + k_{20} \exp\left(-\frac{E_{a2}}{RT}\right)\alpha^m \right](1-\alpha)^n$$

Kinetic parameters determined are:

Curing enthalpy, ΔH = -205 J/g,
Frequency factor k_{10} = 0;
(Activation energy, E_{a1} can be any in this case);
Frequency factor, k_{20} = 12200 s^{-1};
Activation energy, E_{a2} = 51450 J/mol;
Exponent, m = 0.60;
Exponent, n = 1.45;

i.e:

$$\frac{d\alpha}{dt} = 12200 \times \exp\left(-\frac{51450}{RT}\right)\alpha^{0.6} \times (1-\alpha)^{1.45}$$

This equation is what exactly what we need, no more no less — the resin's curing behaviour is fully described. With this equation, one can calculate the curing degree of the resin under any thermal history or curing conditions.

In addition, this DCS approach is a more accurate and better way for determination of thermal properties of a sample, because the intrinsic instrumental deformation of DSC curves have been compensated in the DCS simulations.