# CureKinetics®

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Engineering Research and Flow Technology for Composites



7 avril 2008

# Motivation

Industrial/research requirement for a simple characterization methodology to model resin cure kinetics from DSC measures

# Software goals

1. Accurate numerical solutions for experimental data analysis taking into account trends accuracy and DSC sensitivity

2. Software package for cure kinetics modeling implementing standard models as well as user defined models

3. Creation of glass transition temperature, Inhibition time and gel time models

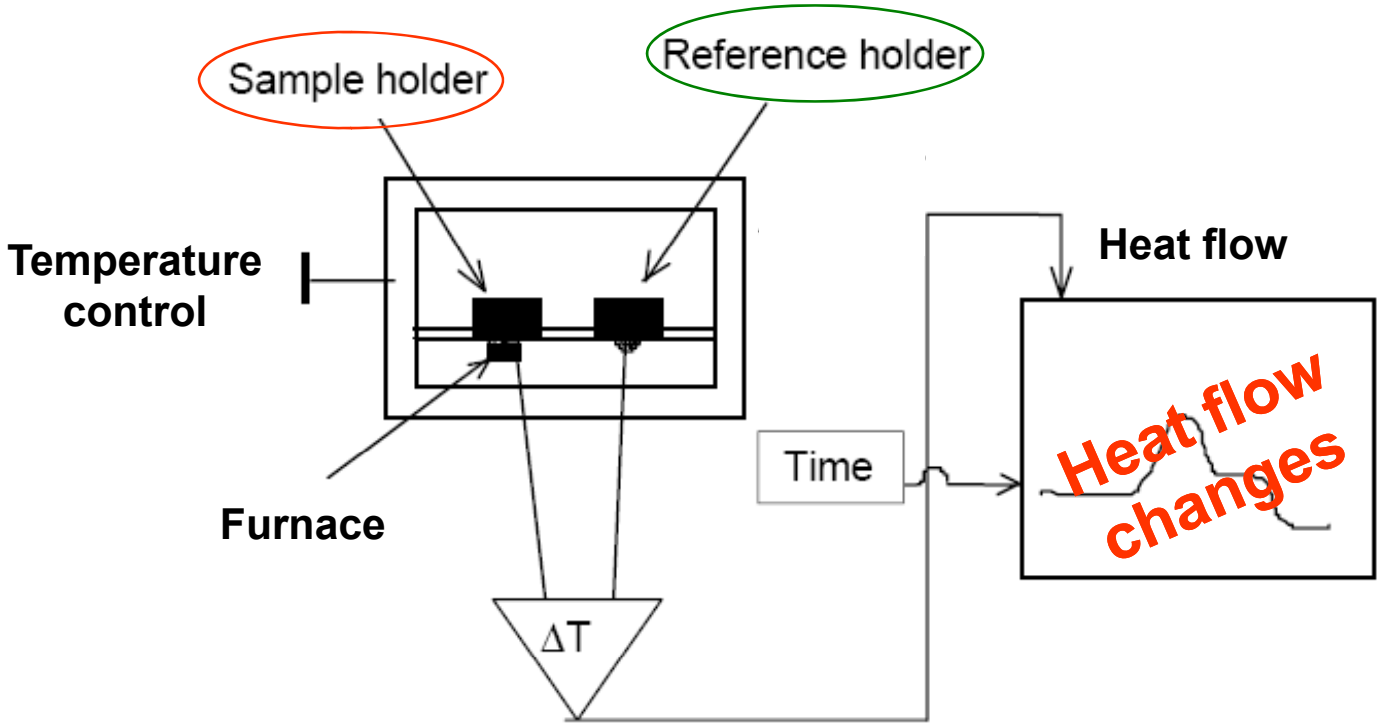
4. Generation of TTT diagrams

5. Prediction of cure evolution for a user defined temperature profile

# Differential Scanning Calorimetry (DSC)

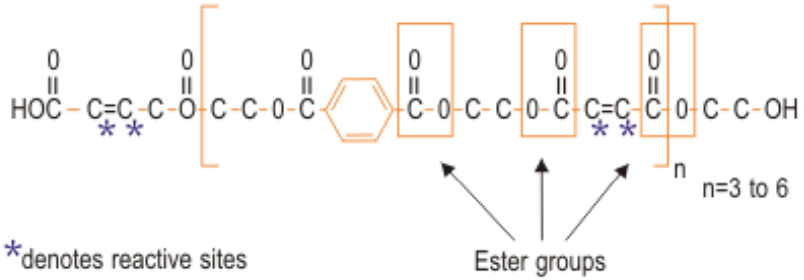
With a DSC instrument phase transitions or chemical reactions in a material can be analyzed when sample is heated, held at a constant temperature or cooled off

**Schematic picture of a DSC instrument**

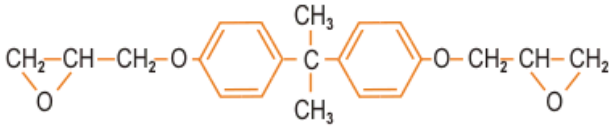


# Polymerization reaction of thermosets

Unsaturated Polyester

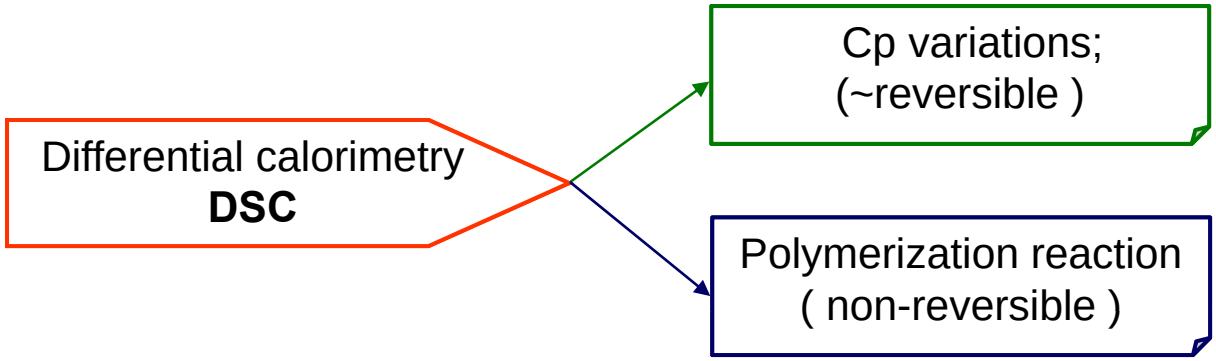



Epoxy



<u>The polymerization reaction is exothermic</u>


Exothermic reaction of unsaturated polyester

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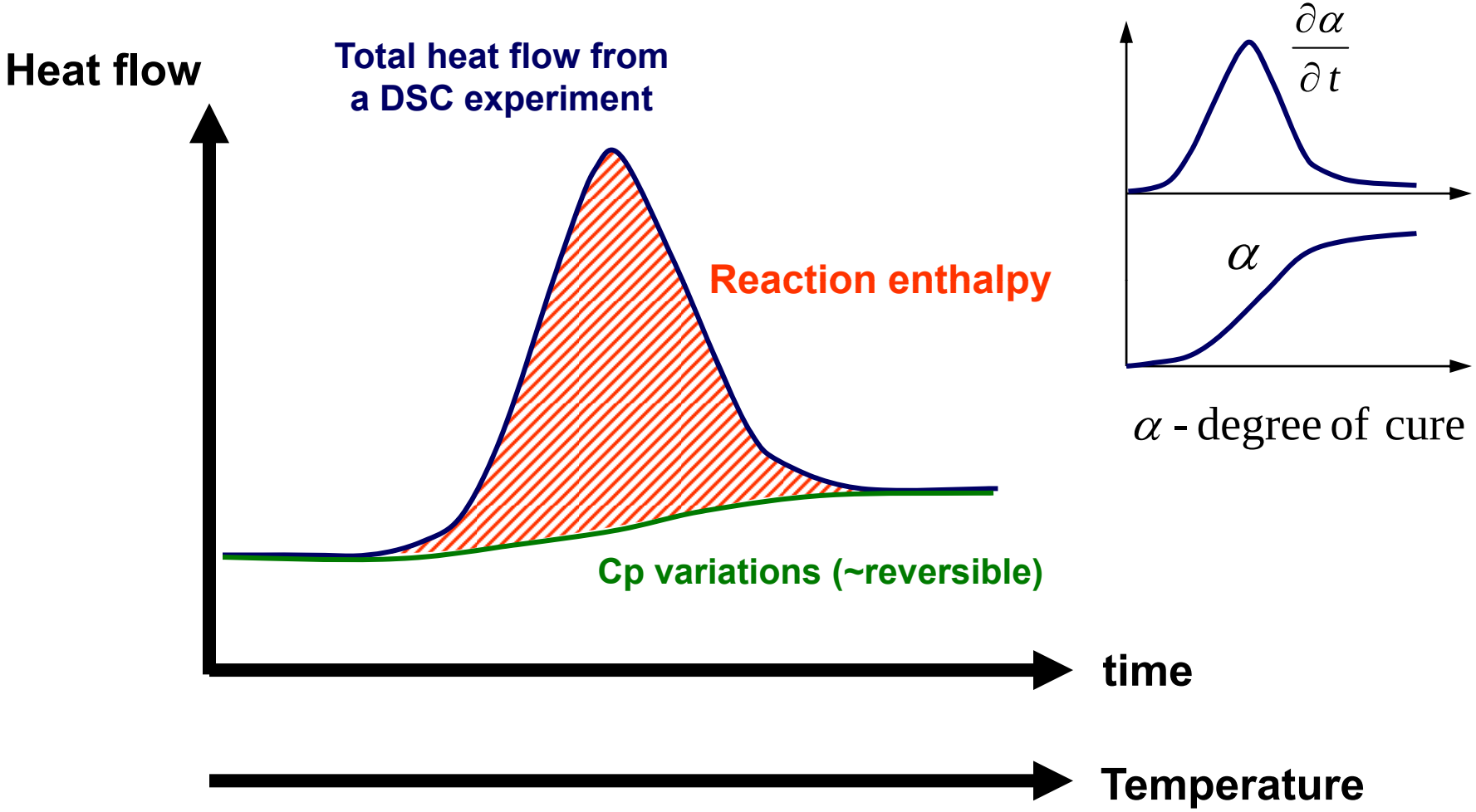
# Polymerization reaction of thermosets



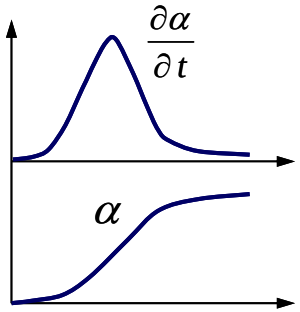
# What *CureKinetics* does?

**DSC data files**

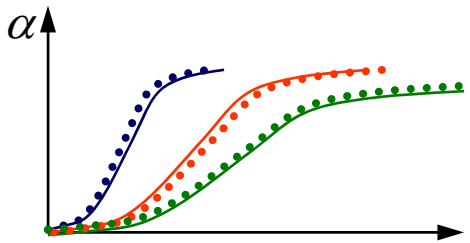
Read

CureKinetics

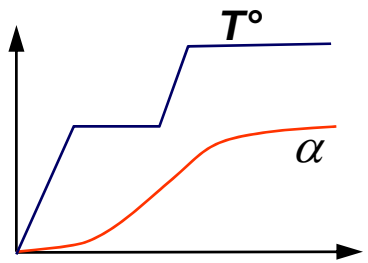
**DSC data analysis**




**Kinetic modeling**



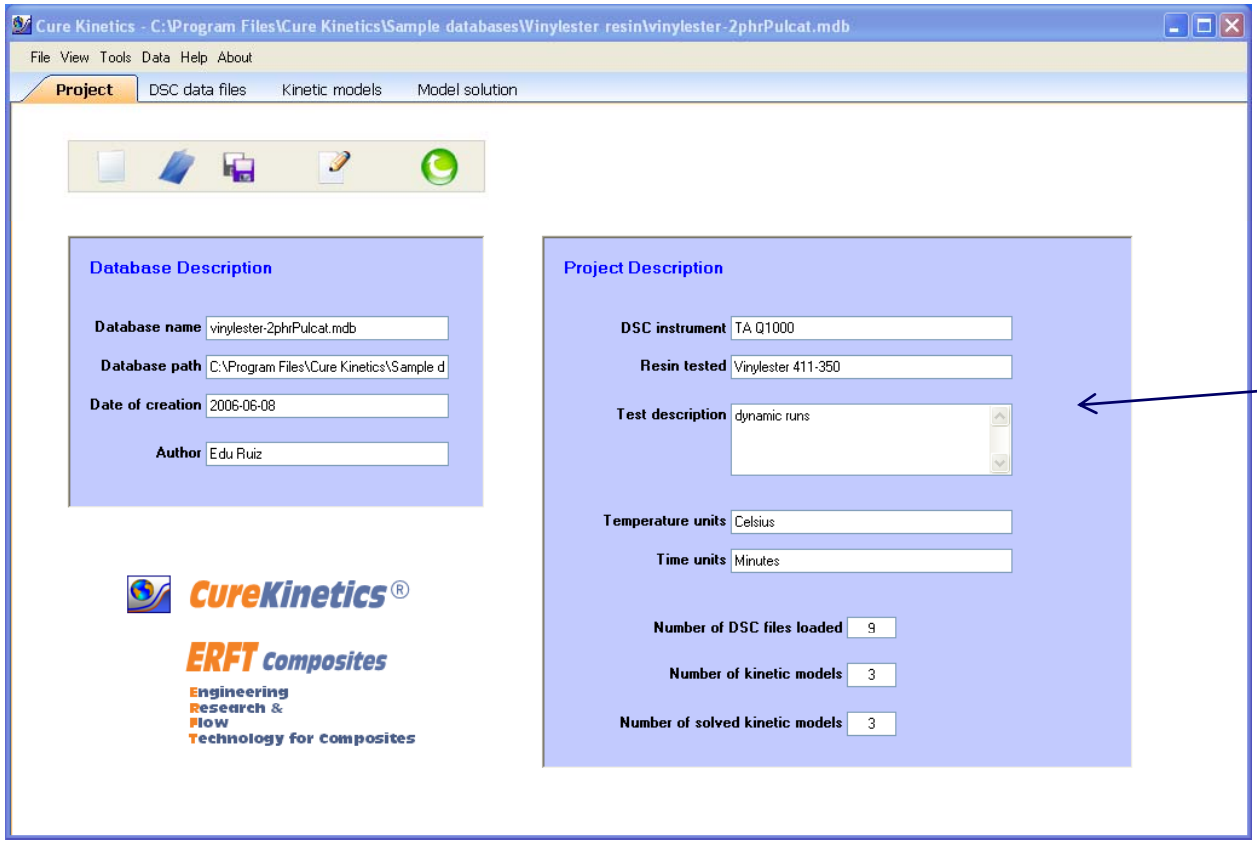

**Cure analysis**




- **Data are stored in a MS Access Database for easy user access**
- **Various kinetic models can be calculated for one set of DSC experiments**
- **Modeling reports can be generated in MS Word**

# How *CureKinetics* looks like?

Startup window




Project description

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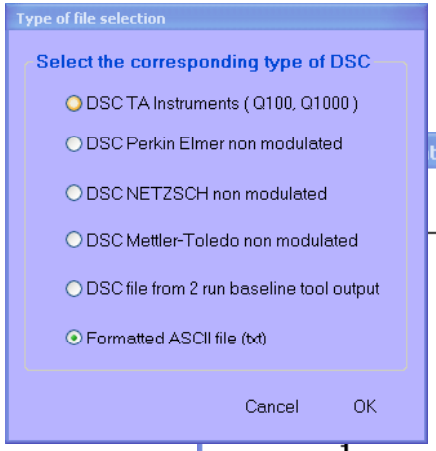
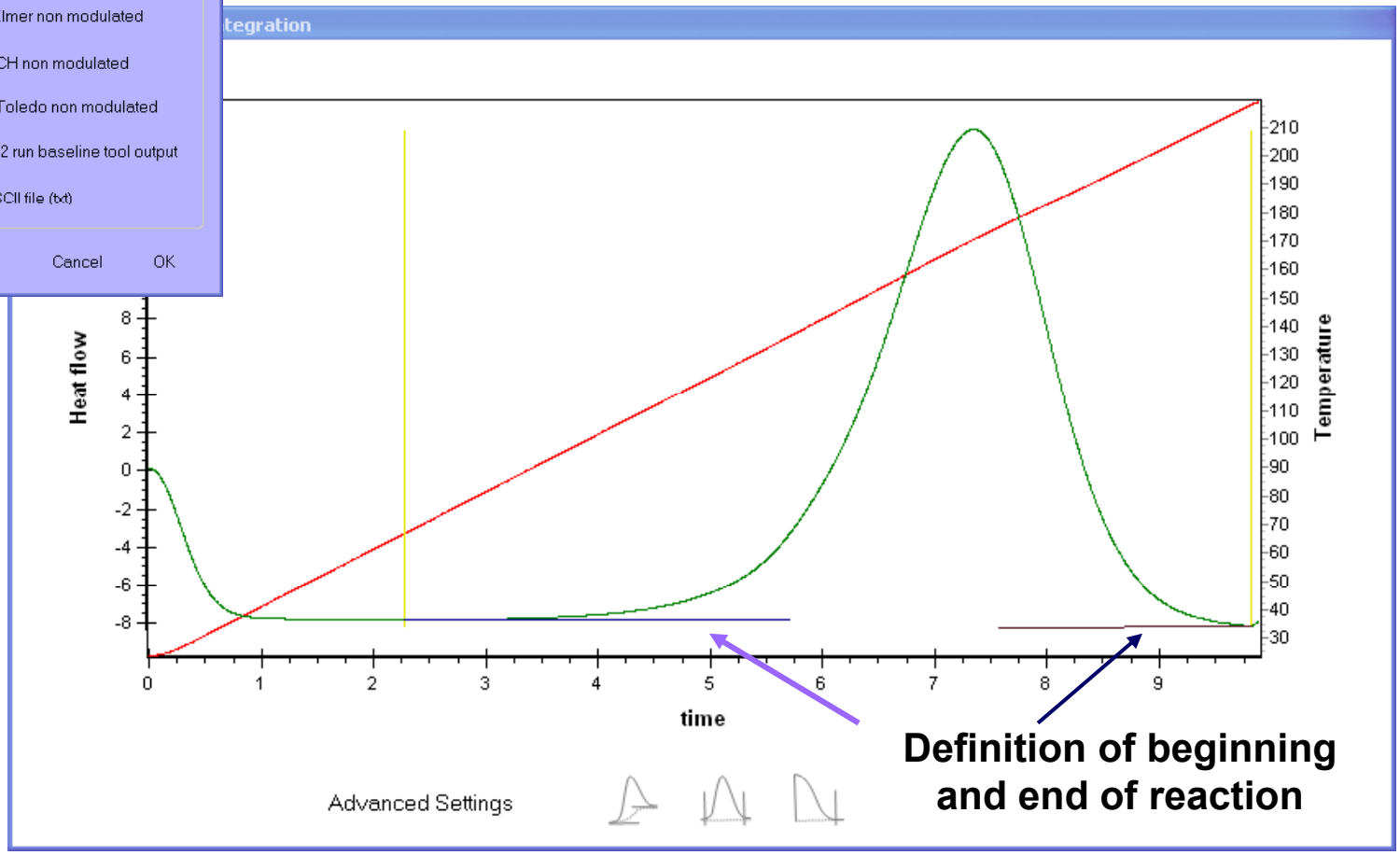
# Loading DSC data files

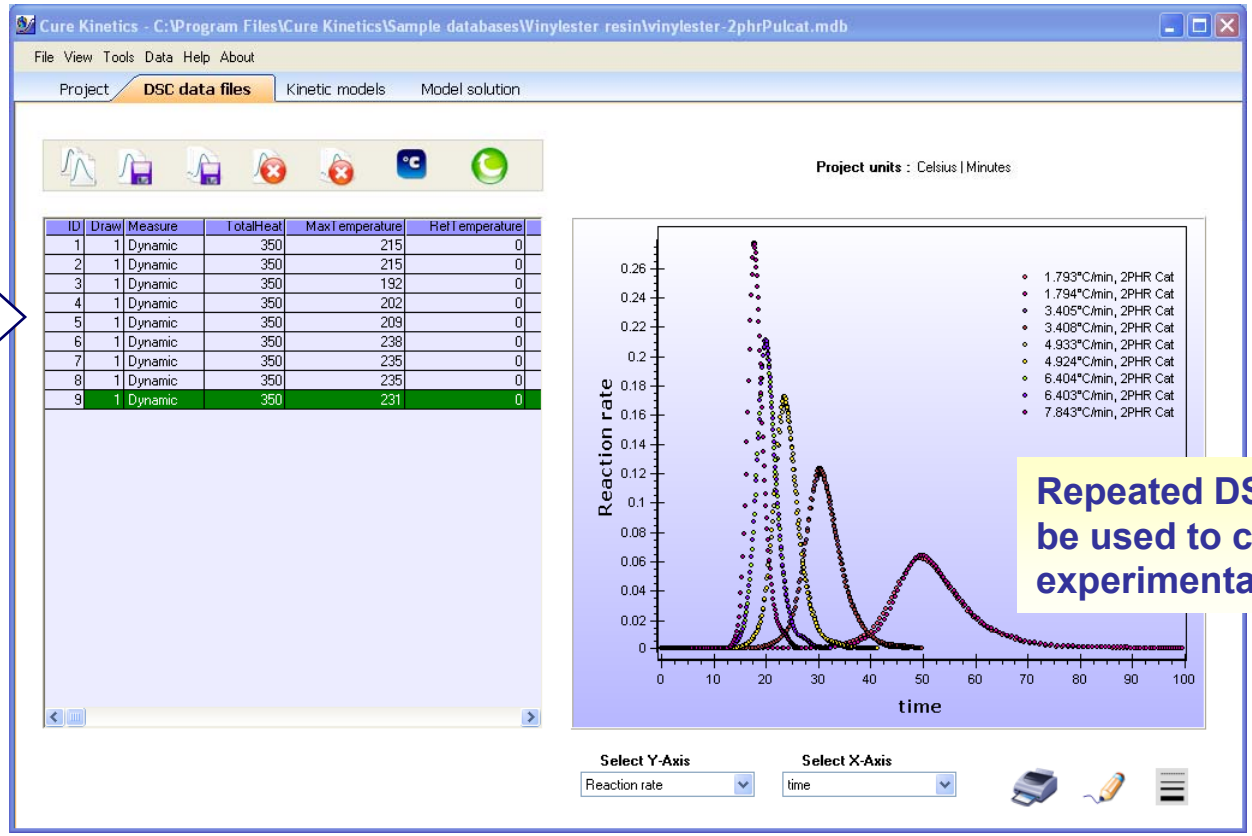
DSC files formats



# DSC data files loaded

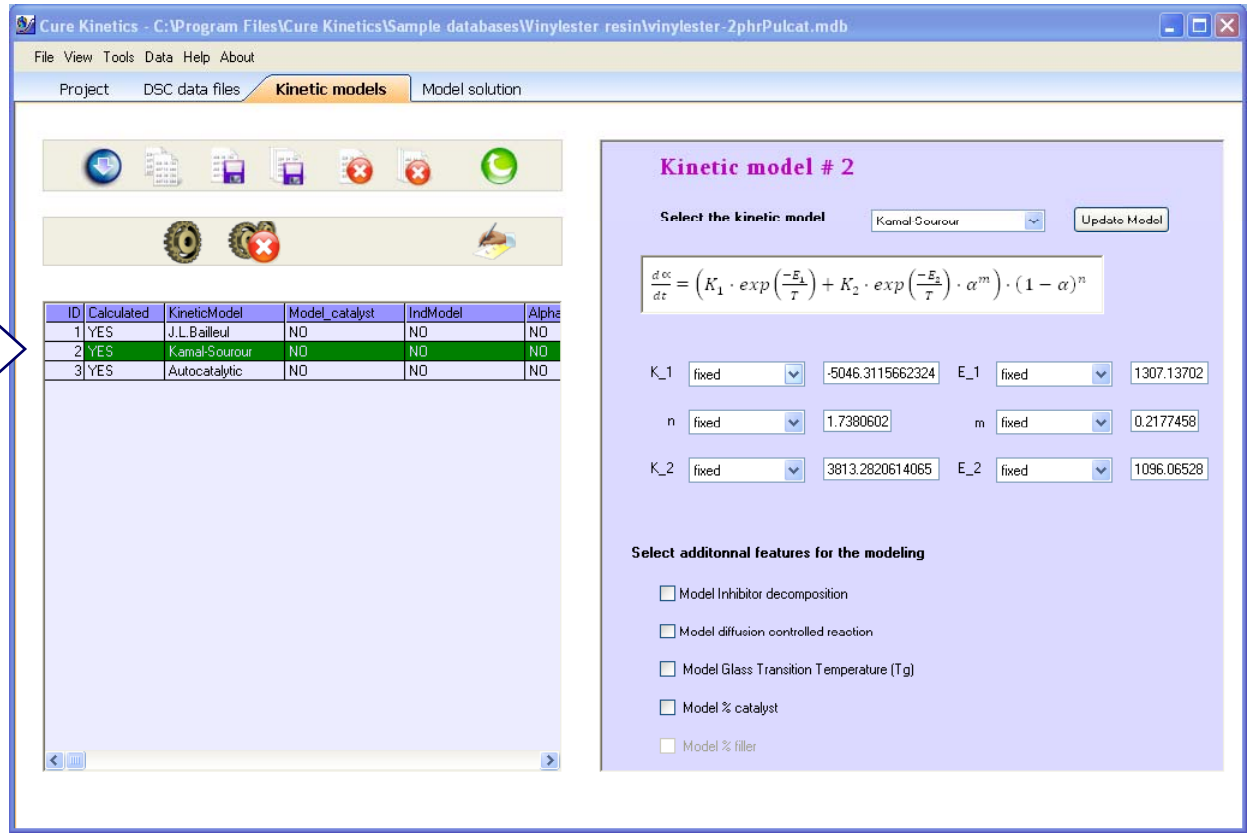
**Series of DSC runs**




**Repeated DSC tests can be used to consider experimental dispersion**

# Definition of kinetic models

**Kinetics models**




**Model parameters**

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# Available kinetic models

Autocatalytic $$\frac{d\alpha}{dt} = K_1 \cdot exp\left(\frac{-E_1}{T}\right) \cdot \alpha^m \cdot (\alpha_{max}(T) - \alpha)^n \cdot F(\alpha)$$

Kamal-Sourour $$\frac{d\alpha}{dt} = \left(K_1 \cdot exp\left(\frac{-E_1}{T}\right) + K_2 \cdot exp\left(\frac{-E_2}{T}\right) \cdot \alpha^m\right) \cdot (\alpha_{max}(T) - \alpha)^n \cdot F(\alpha)$$

Ruiz $$\frac{d\alpha}{dt} = K_1 \cdot exp\left(-E_1\left(\frac{T_{ref}}{T} - 1\right)\right) \cdot G(\alpha) \cdot (\alpha_{max}(T) - \alpha)^n \cdot F(\alpha)$$

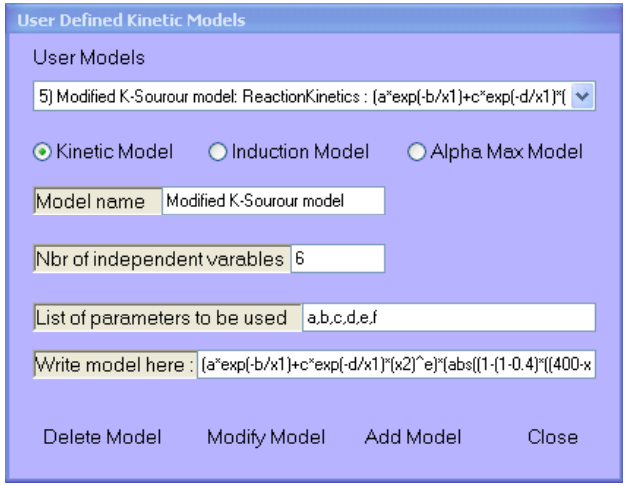
J.L. Bailleul $$\frac{d\alpha}{dt} = K_1 \cdot exp\left(-E_1\left(\frac{T_{ref}}{T} - 1\right)\right) \cdot G(\alpha) \cdot F(\alpha)$$

nth-order $$\frac{d\alpha}{dt} = K_1 \cdot exp\left(\frac{-E_1}{T}\right) \cdot (\alpha_{max}(T) - \alpha)^n \cdot F(\alpha)$$

Mechanistic $$\frac{d\alpha}{dt} = K_3 exp\left(\frac{-E_3}{T}\right) \cdot I_0 \cdot (\alpha_{max}(T) - \alpha) \cdot \beta \cdot F(\alpha)$$
$$\frac{d\beta}{dt} = K_1 exp\left(\frac{-E_1}{T}\right) - \left[K_1 \cdot exp\left(\frac{-E_1}{T}\right) + K_2 \cdot exp\left(\frac{-E_2}{T}\right)\right] \cdot \beta$$

Diffusion $$F(\alpha) = \frac{1}{1 + exp(E_1(\alpha - \alpha_c))}$$

**User defined models**

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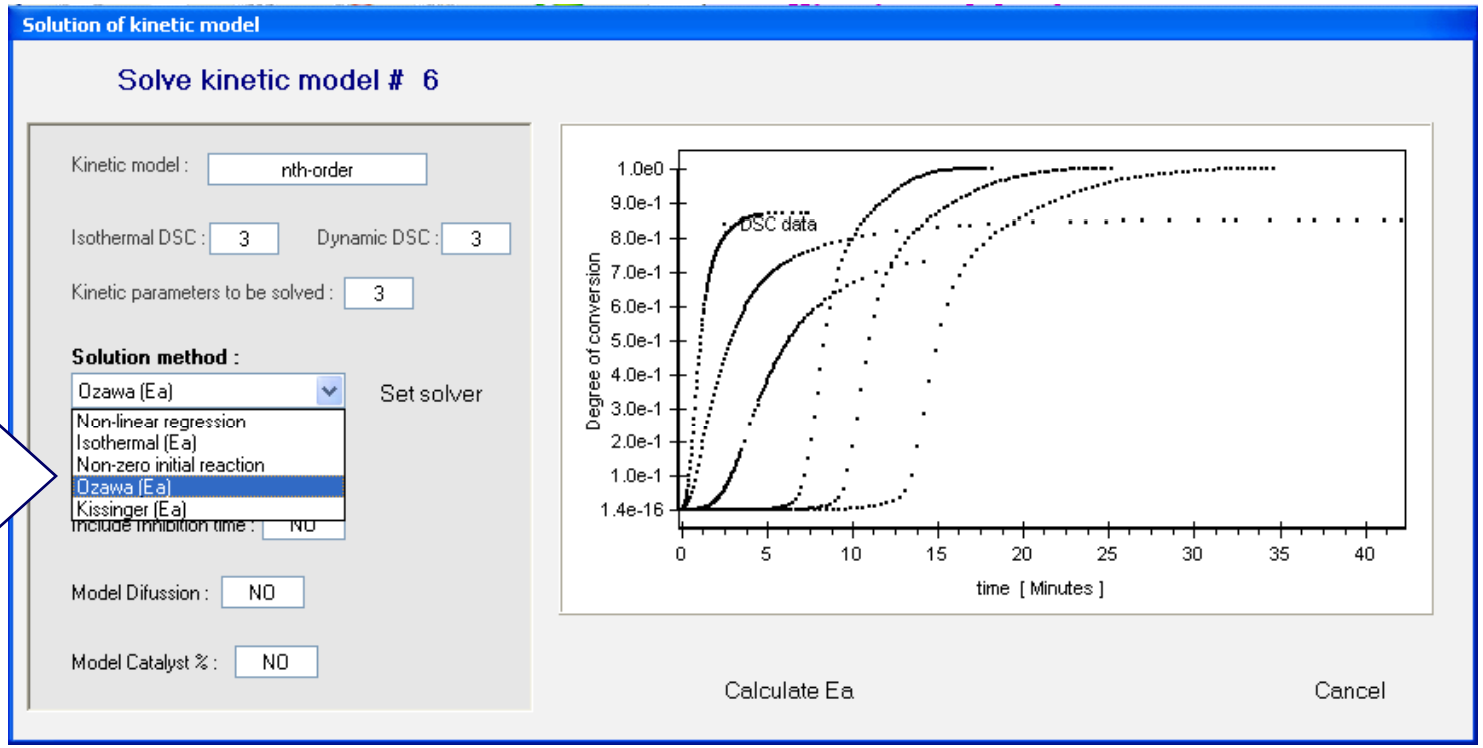
# Solution of kinetic models




**Solution methods**

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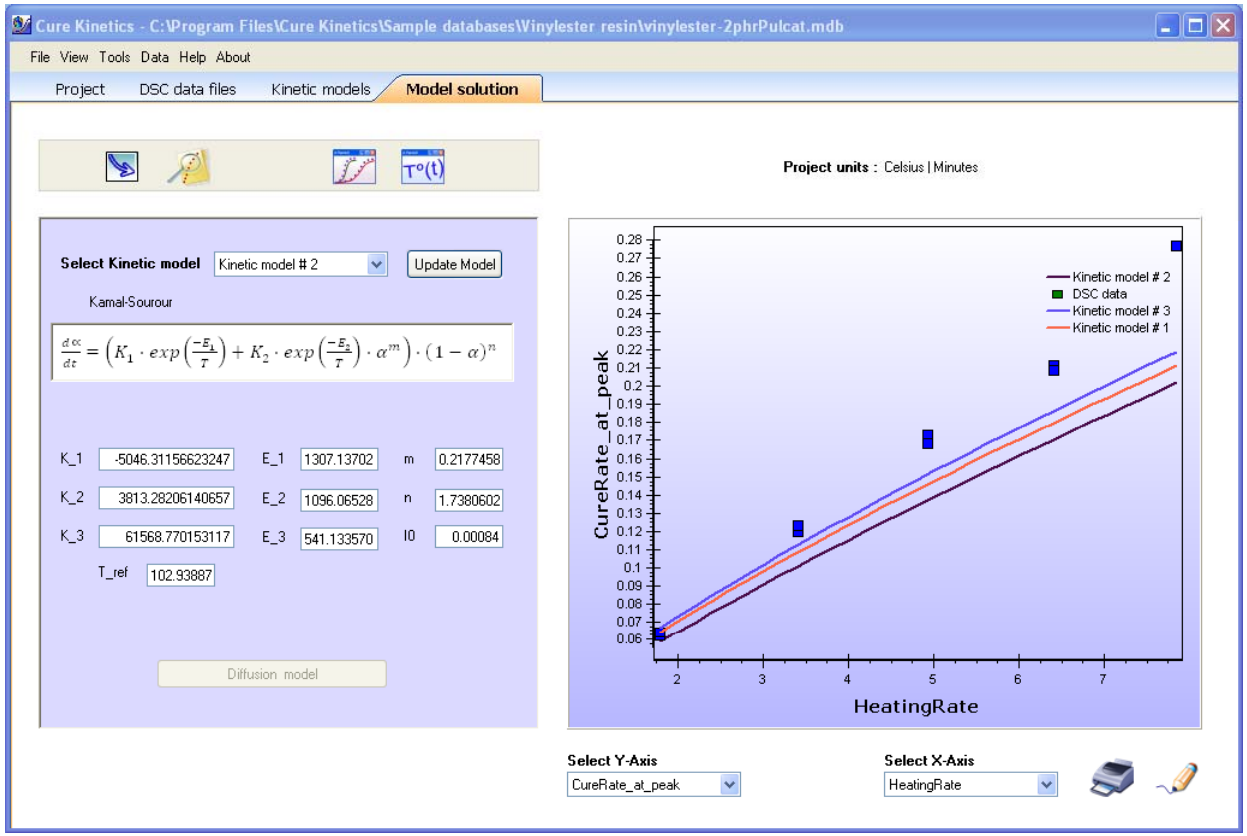
# Verification of kinetic parameters (rate at peak, cure al peak, etc)

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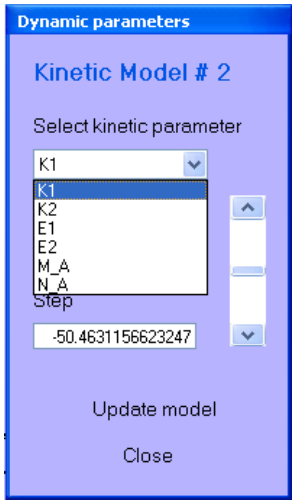
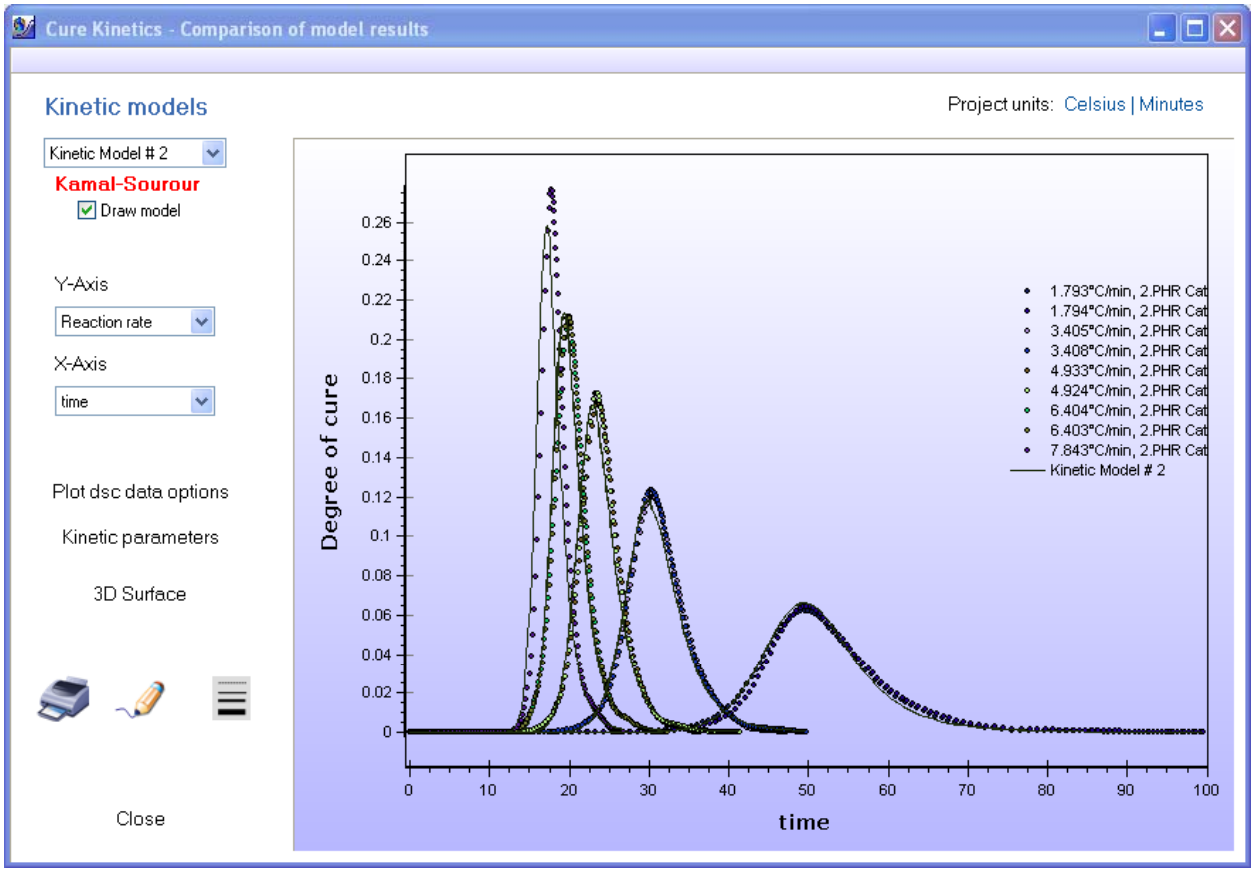
# Comparison of kinetic models and DSC data

**Dynamic correction of model parameters**

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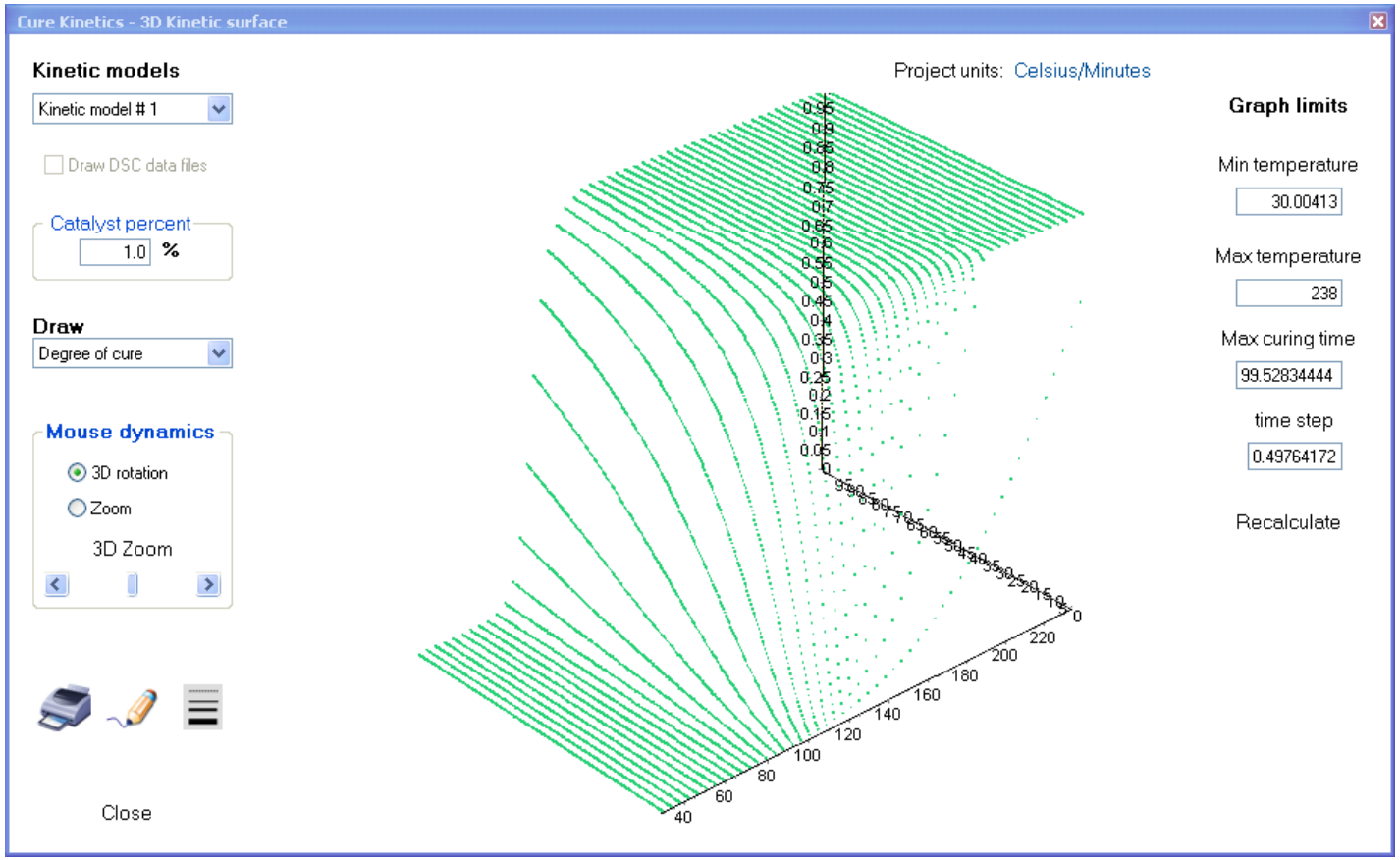
# 3D graphs of kinetic models

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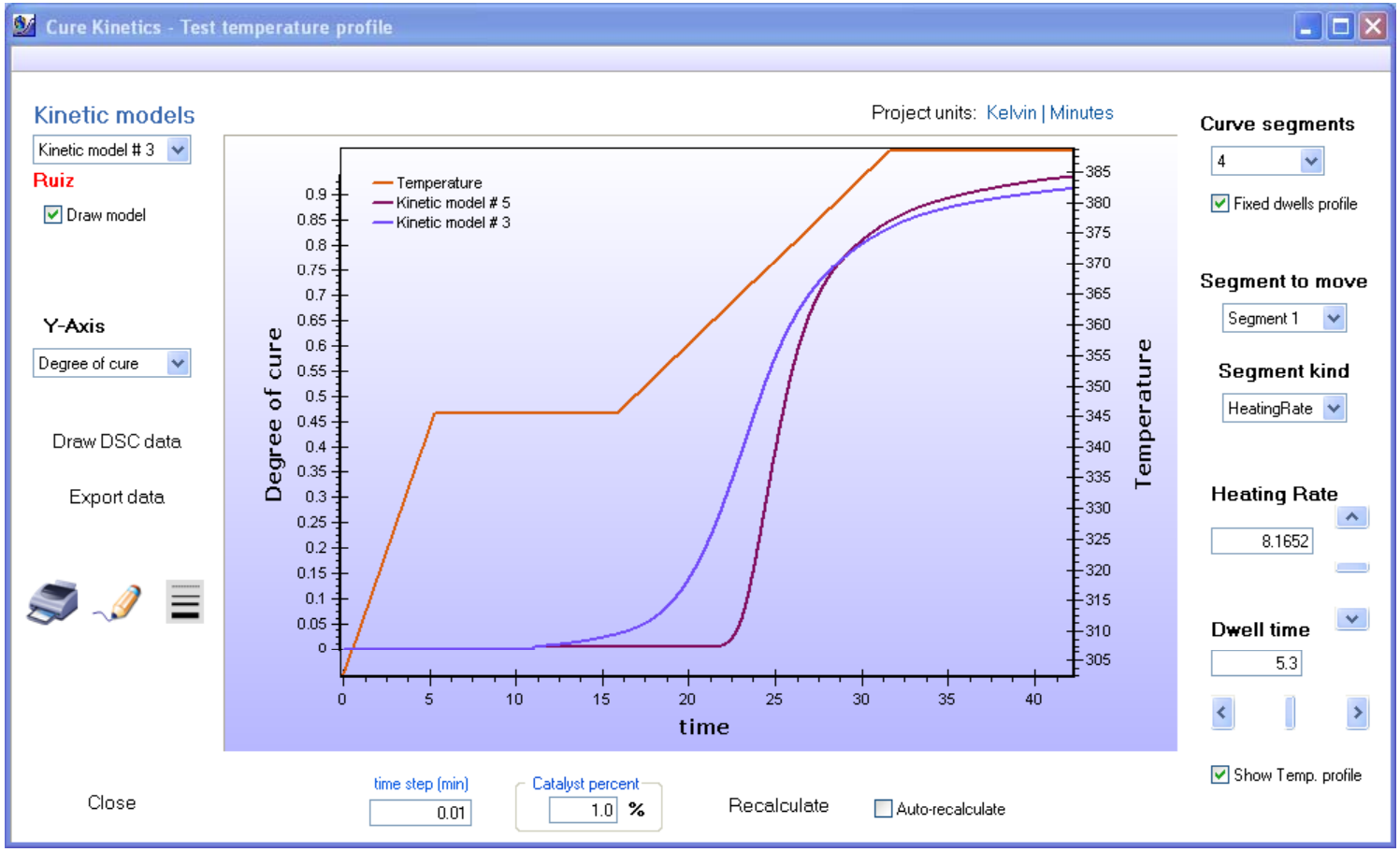
# Model solution for a temperature profile

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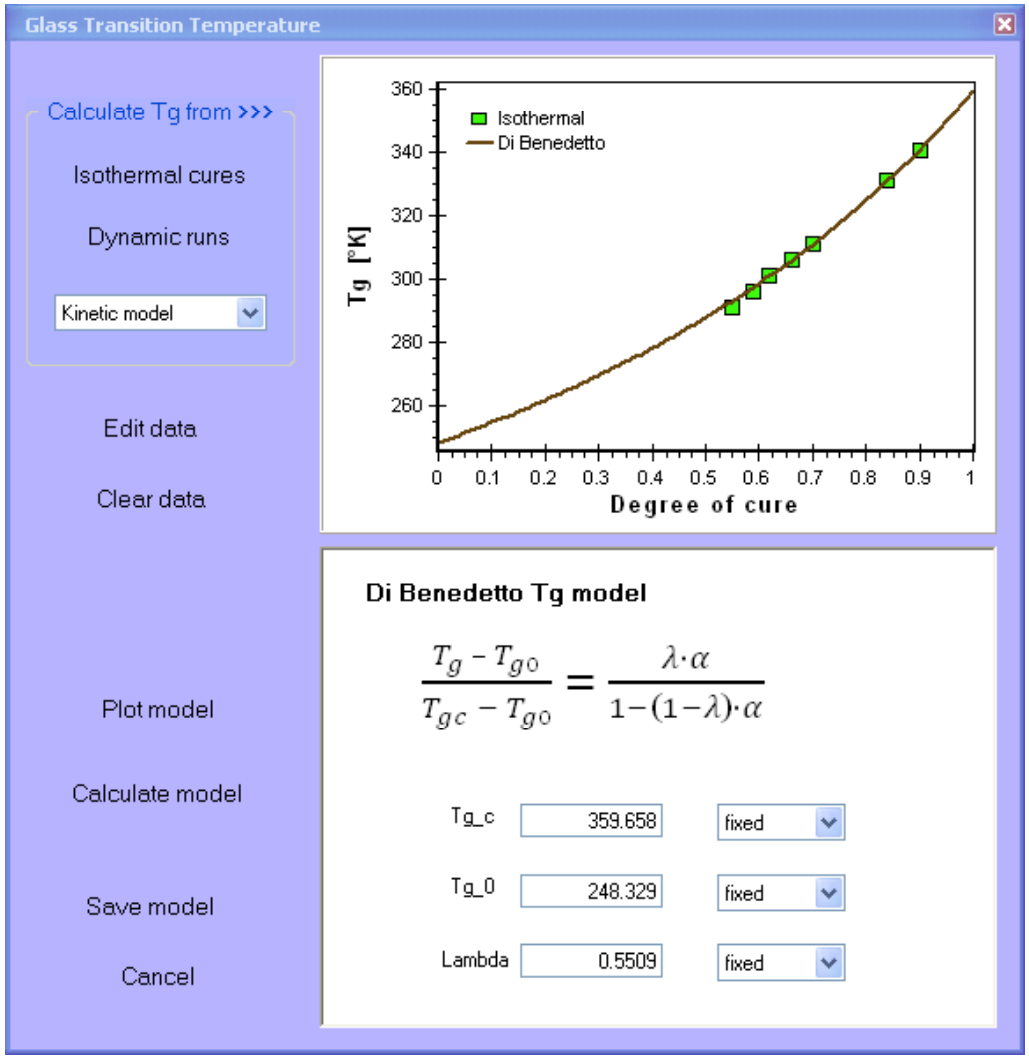
# Glass transition temperature

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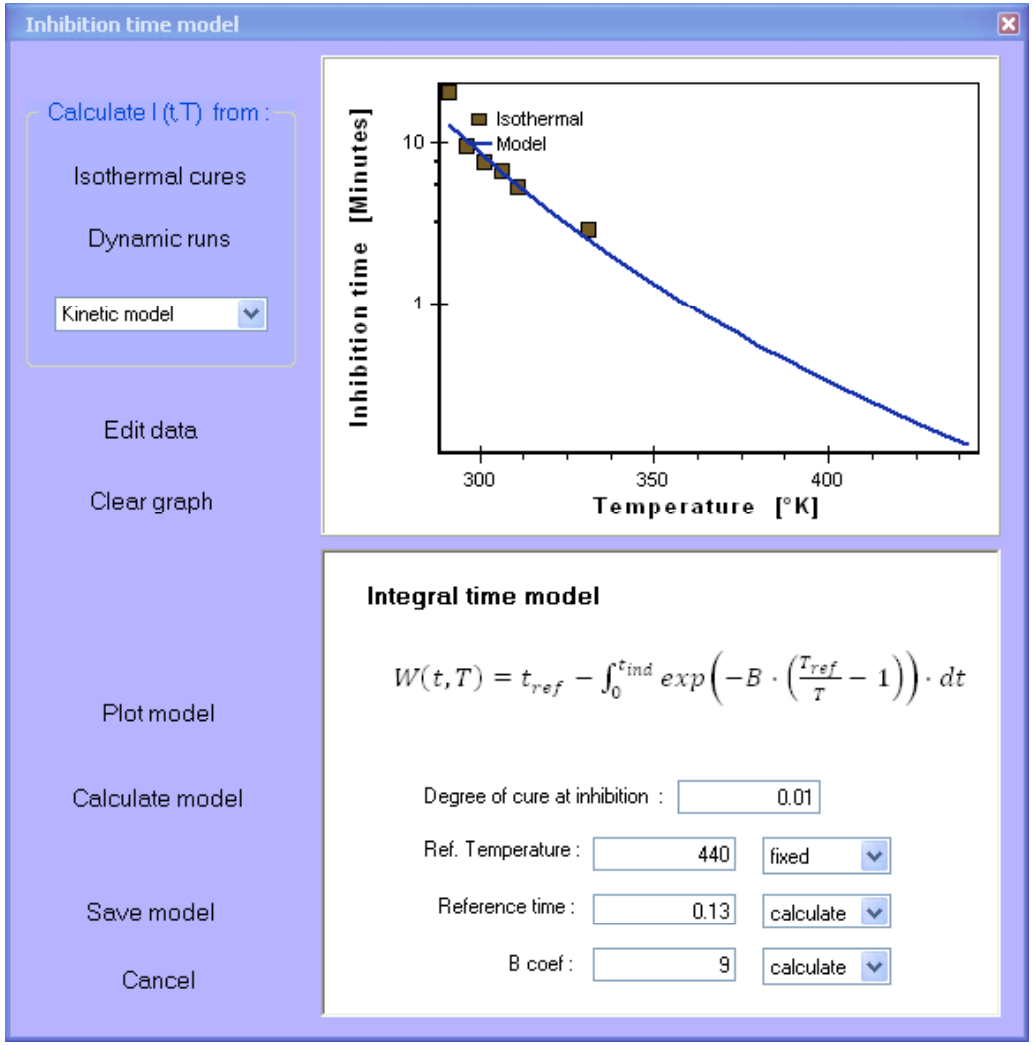
# Inhibition time model

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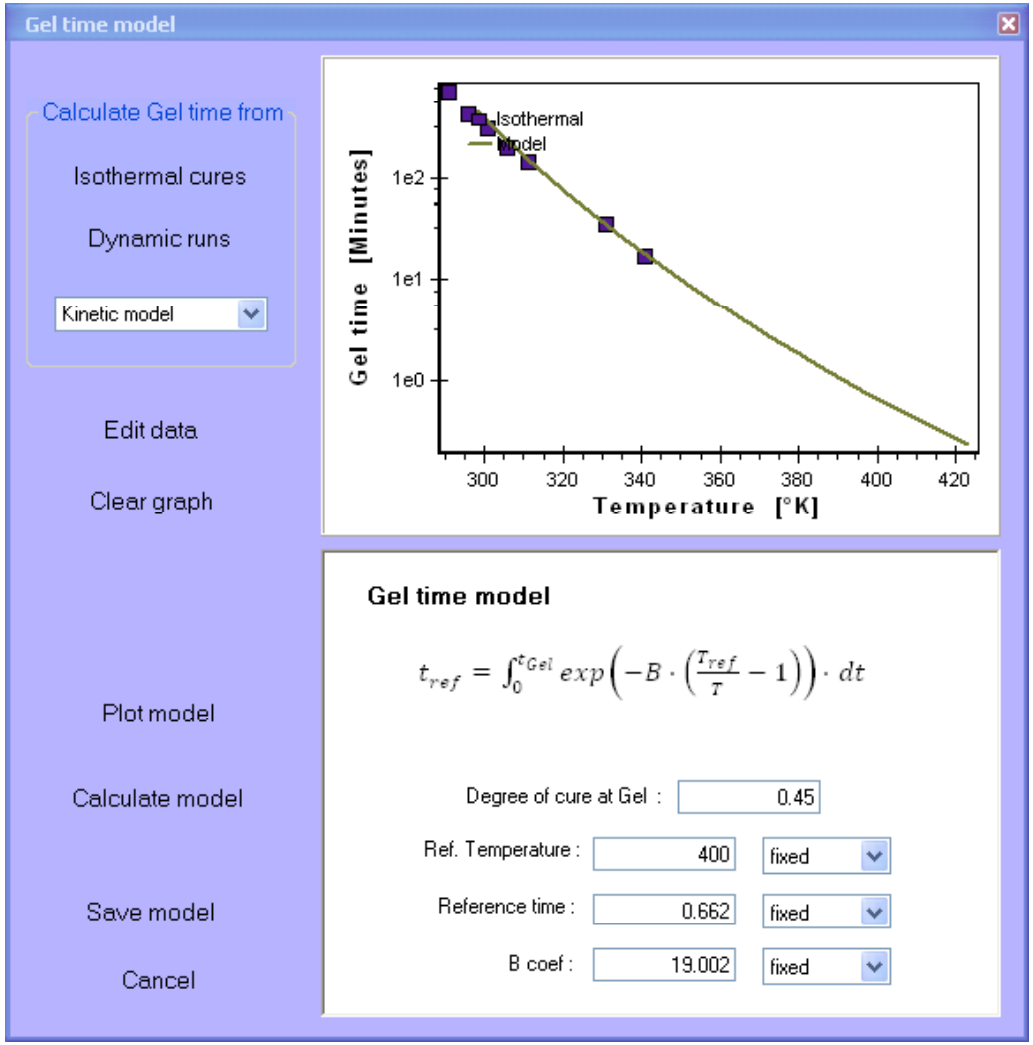
# Gel time model

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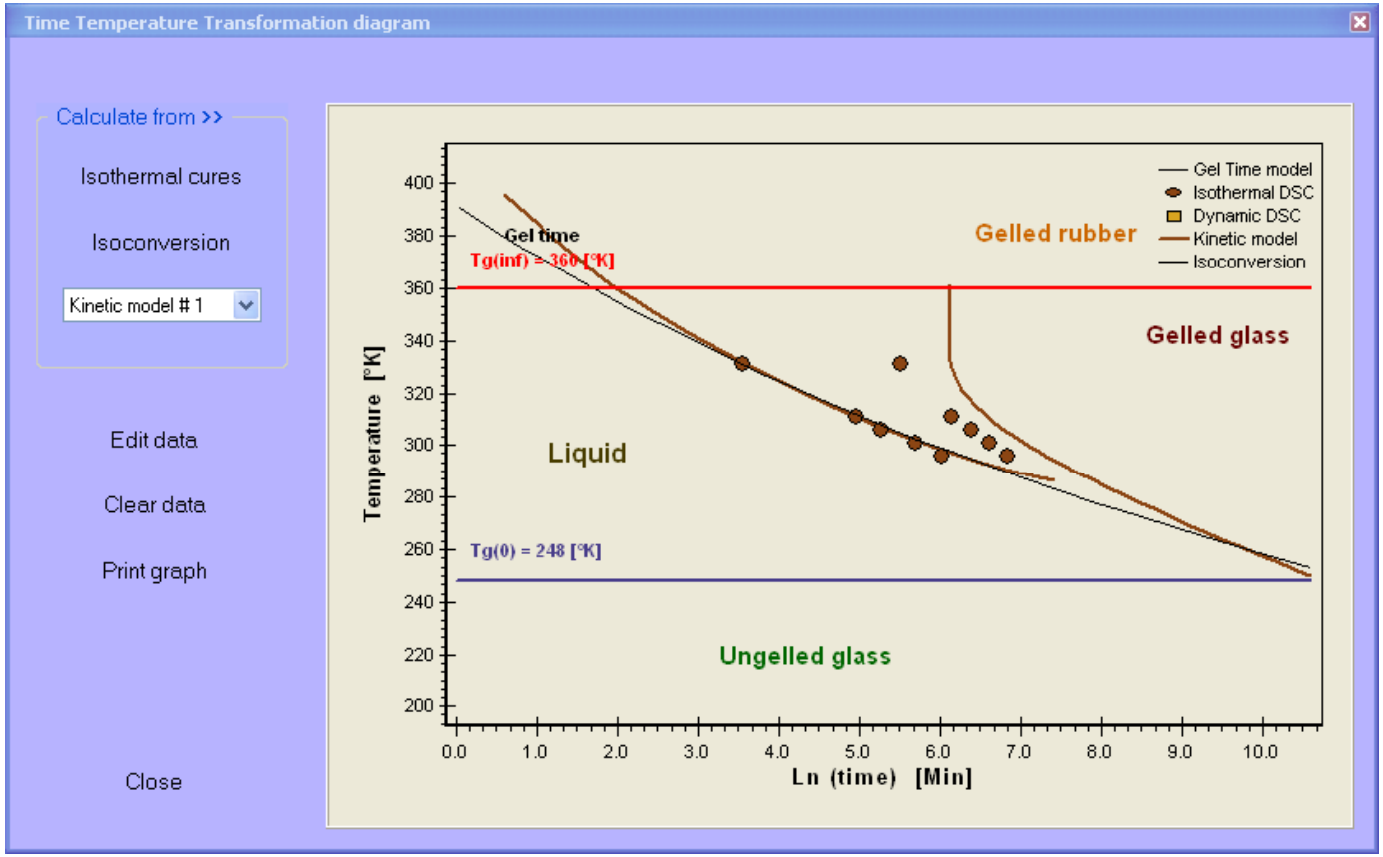
# Time-Temperature-Transformation diagram

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