Analyzing & Testing

KINETICS NEO

NETZSCH

Proven Excellence.

Advantages and disadvantages of different thermokinetic approaches
Unique and powerful features of Kinetics Neo Software

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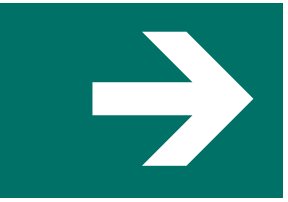
NETZSCH Webinar – 29th April 2021

Agenda

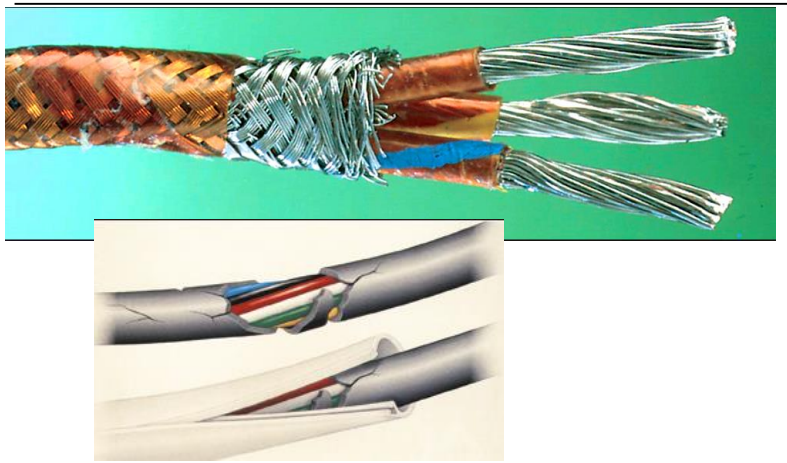
1. Target of thermokinetic analysis
    - 1.1 Brief overview
    - 1.2 Measurements for kinetic analysis
2. How to solve the problems? Different analysis approaches
    - 2.1 Degree of conversion
    - 2.2 Arrhenius equation, activation energy, kinetic triplet
    - 2.3 Overview of the model-free and model based approaches.
    - 2.4 Why model-free is often not applicable.
    - 2.5 Advantages and disadvantages
    - 2.6 Limitations of solutions and prediction
3. Unique Features of Kinetics Neo Software
    - 3.1 Fulfils all ICTAC kinetic recommendations
    - 3.2 Numerical model free method
    - 3.3 Special functions for curing
        - 3.3.1 Kamal-Sourour autocatalytic model
        - 3.3.2 Diffusion control, vitrification and TTT diagram
        - 3.3.3 Kinetic analysis of rheological data and prediction of dynamic viscosity
    - 3.4 Crystallization kinetics
    - 3.5 Multi-step model based method, including presentation of each individual reaction step
    - 3.6 Small other features (Bezier baseline, export equations…)



1. Target of thermokinetics analysis

Brief overview of the problems solving by thermokinetics

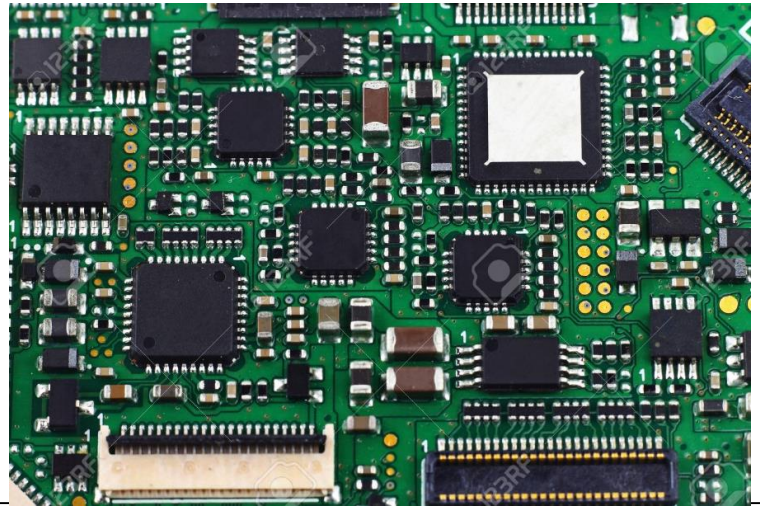
1.1 Application fields



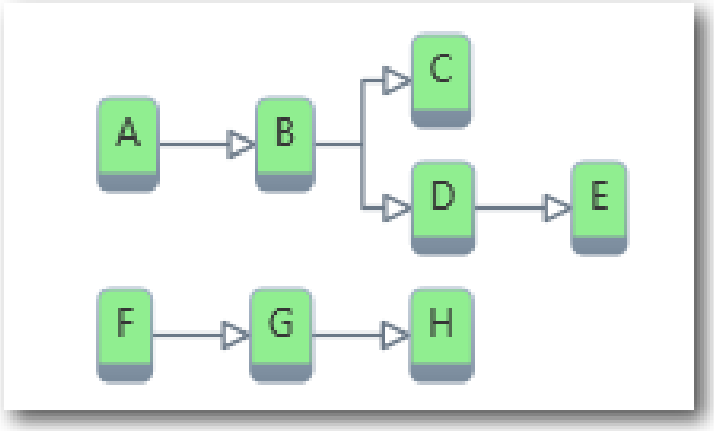
Life time predictions
Recycling, pyrolysis
Thermal stability

Curing, cross-linking

Sintering, ceramics



1.1 Purposes of kinetic analysis



A → B

reactant product

Academic

*Chemical mechanism is the **subject** of study*

- **Find** and describe the kinetic **mechanism**

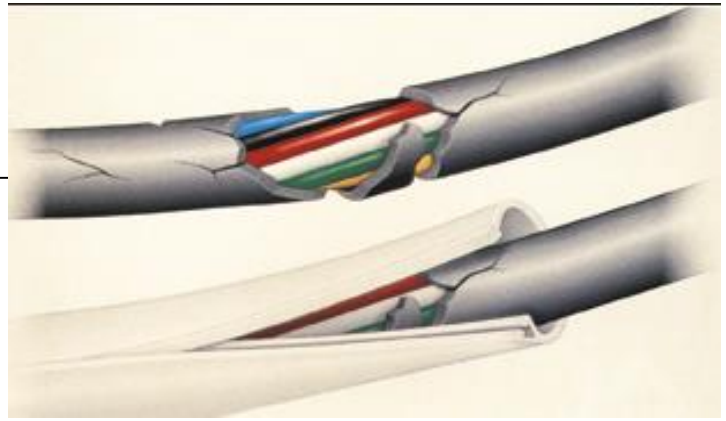
Industrial

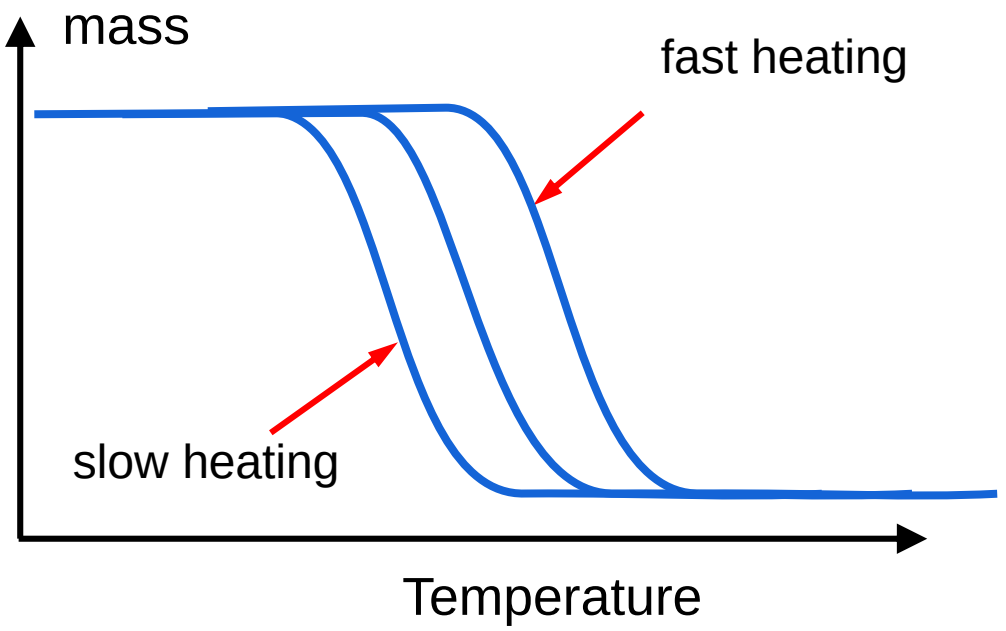
*Chemical mechanism of reaction is **unknown** or **not important***

- **Predict** conversion(Temp,time) and reaction rate for given temperature program

- **Optimize** industrial processes: decrease production time and costs and improve the quality of product

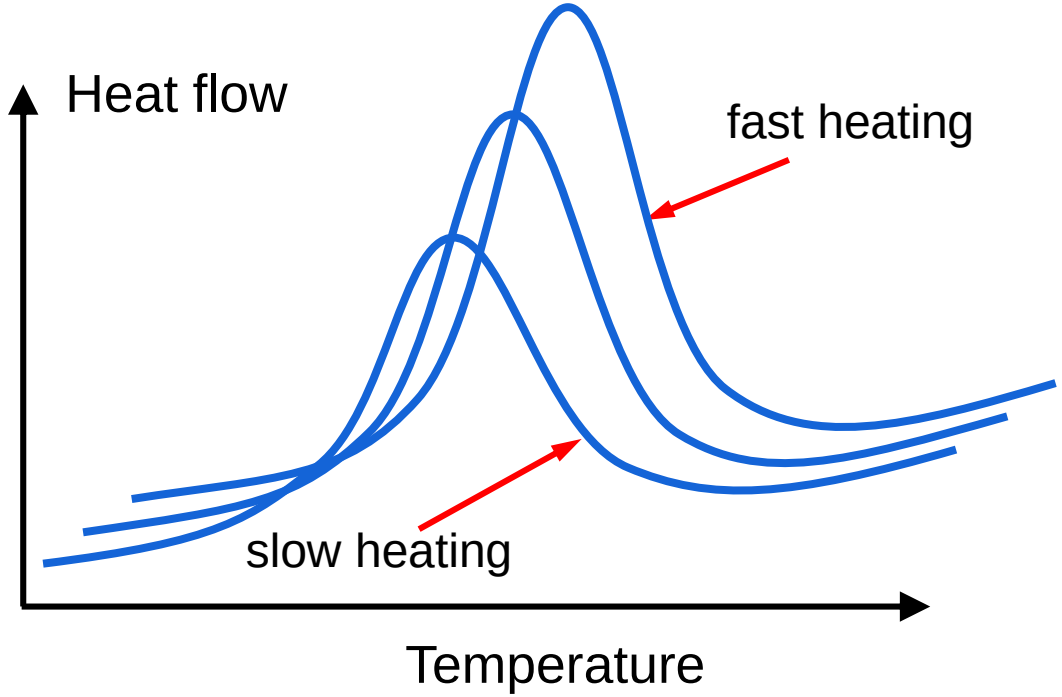
1.2 Measurements for kinetic analysis: Thermogravimetry





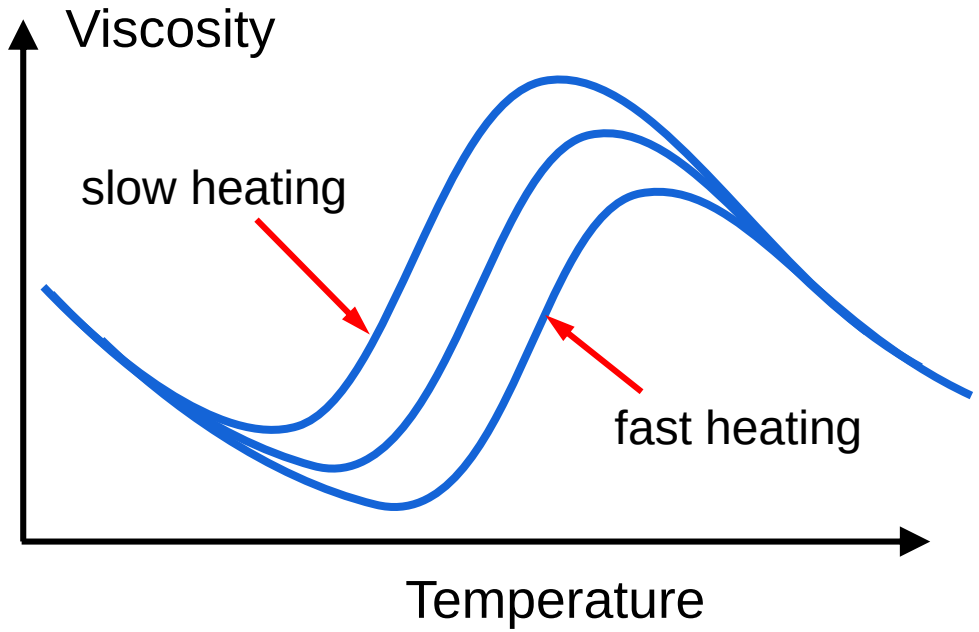
Thermogravimetry: mass change is measured during heating

1.2 Measurements for kinetic analysis: Differential scanning calorimetry



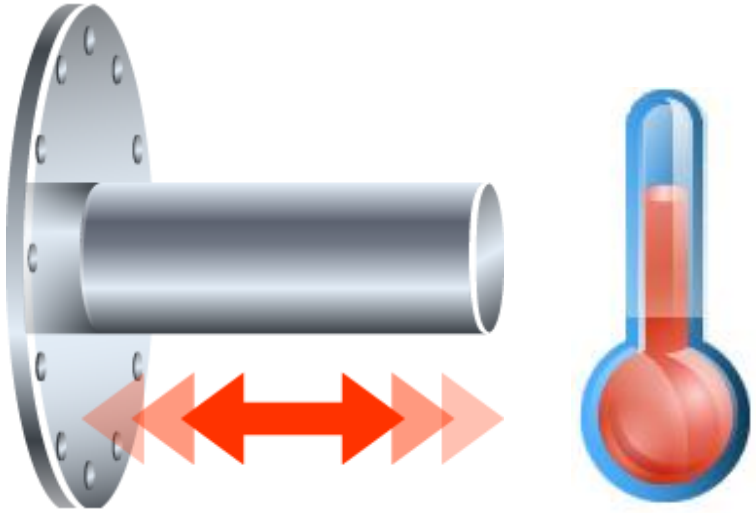
Differential scanning calorimetry: heat flow is measured during temperature

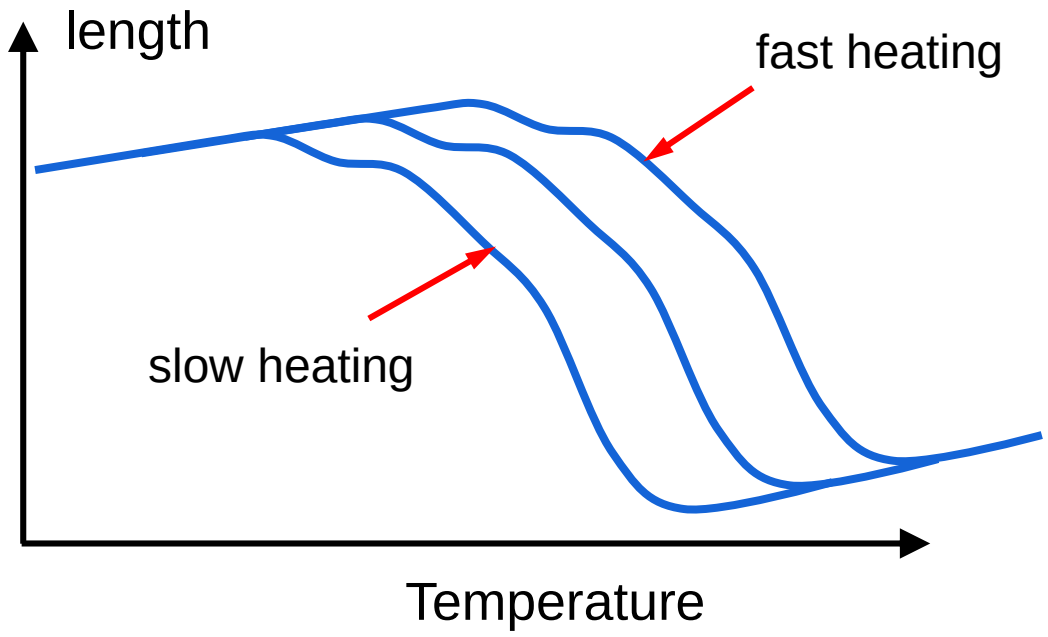
1.2 Measurements for kinetic analysis: Rheometry



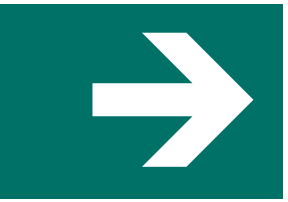
Rheometry: viscosity is measured during temperature

1.2 Measurements for kinetic analysis: Dilatometry





Dilatometry: length change is measured during heating

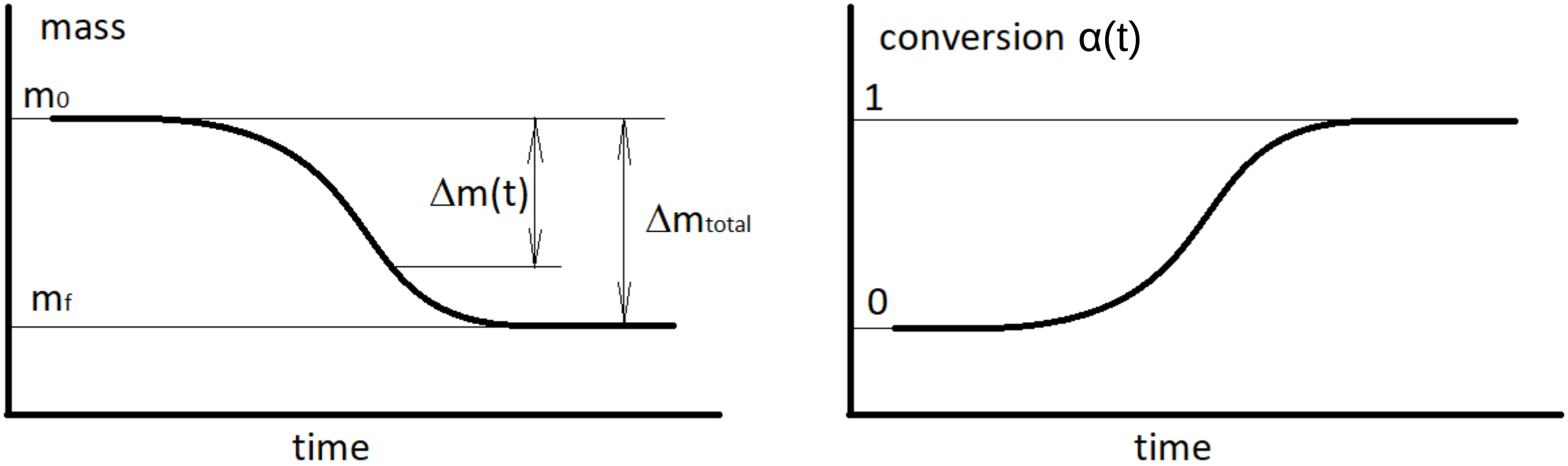


2. Different analysis approaches

Different approaches, advantages, disadvantages, limitations

2.1 Degree of conversion α(t) for TGA data (extent of conversion, conversion, extent of reaction)

Commonly denoted by **α** and defined as the ratio of the partial to total change of a physical property.

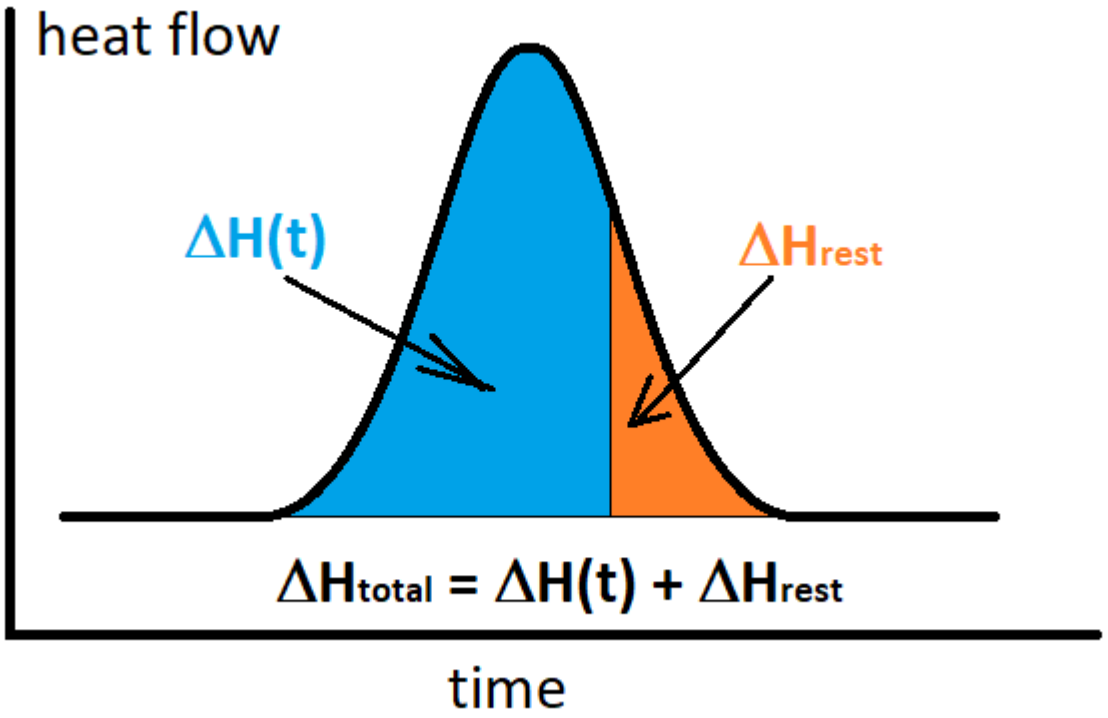


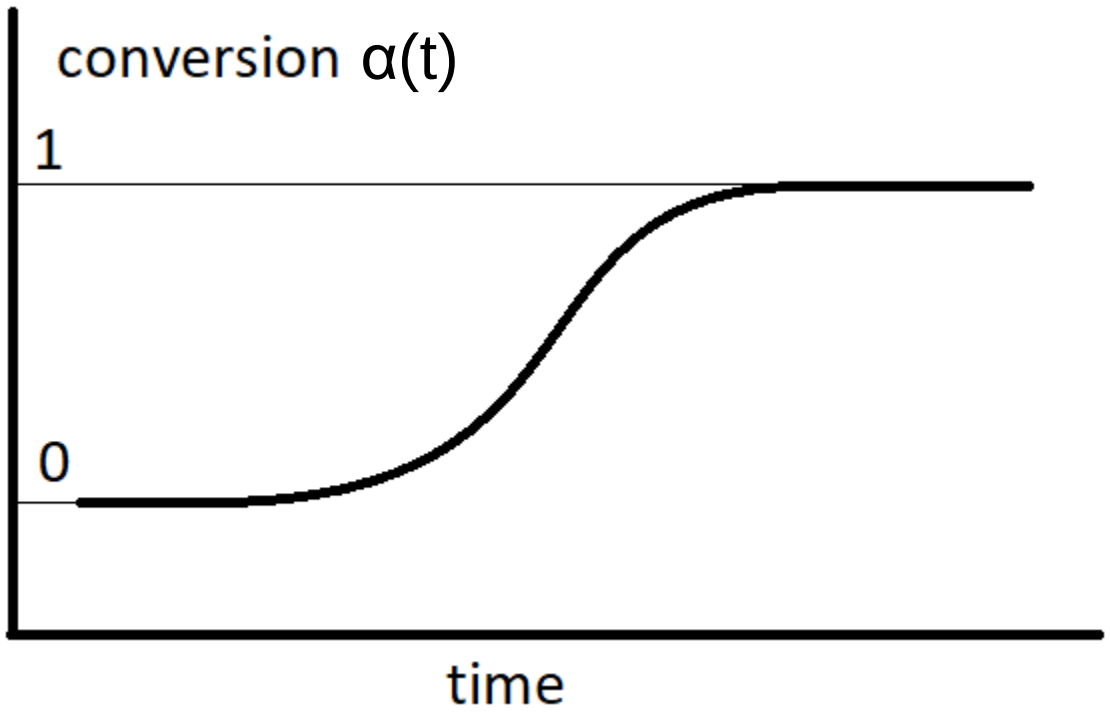
$$\alpha(t) = \frac{\Delta m(t)}{\Delta m_{total}}$$

α=0 before reaction start
α=1 after reaction end

TGA: Conversion is the **ratio of the partial mass loss** at given time point **to the total mass loss** at the final time point

2.1 Conversion α(t) for DSC data

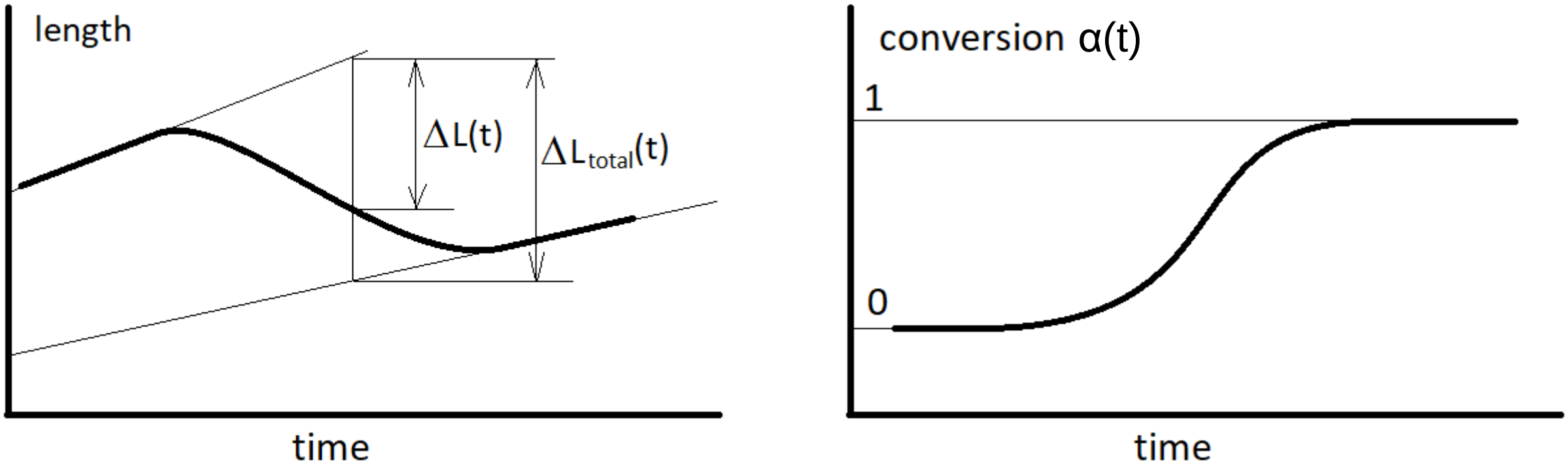




$$\alpha(t) = \frac{\Delta H(t)}{\Delta H_{total}}$$

DSC: Conversion is the ratio of the partial enthalpy change at given time point **to the total enthalpy change** at the final time point

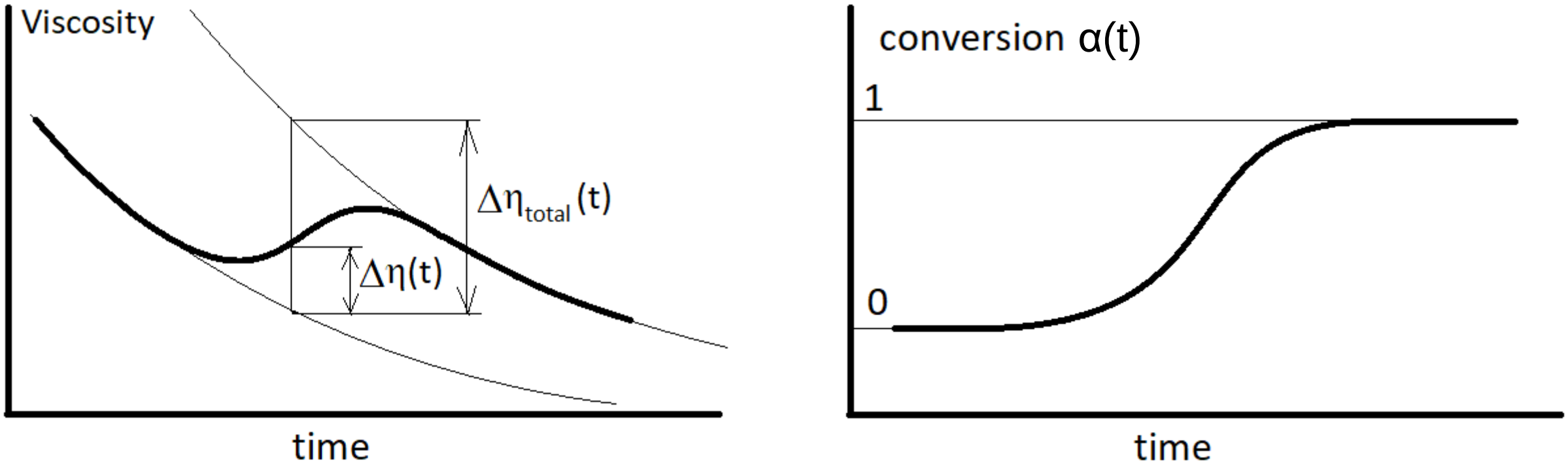
2.1 Conversion α(t) for dL data during heating



$$\alpha(t) = \frac{\Delta L(t)}{\Delta L_{total}(t)}$$

DIL: Conversion is the ratio of the partial length change at given time point **to the total length change** between extrapolated baselines at the this point

2.1 Conversion α(t) for viscosity data during heating



$$\alpha(t) = \frac{\Delta\eta(t)}{\Delta\eta_{total}(t)}$$

Viscosity: Conversion is the ratio of the partial viscosity change at given time point **to the total viscosity change** between extrapolated baselines at the this point

Steps to solve Kinetic Tasks in Kinetics Neo

Measured raw data

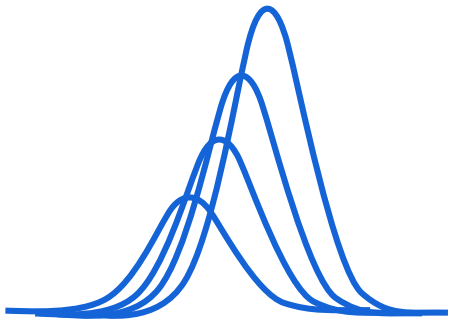
File 1

File 2

File 3

File 4

...



Data Import and Processing

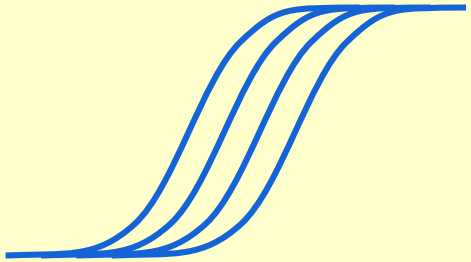
Processed File 1

Processed File 2

Processed File 3

Processed File 4

...



Kinetic Model / Method

Autocatalytic (Cn)

Reaction of n-th order

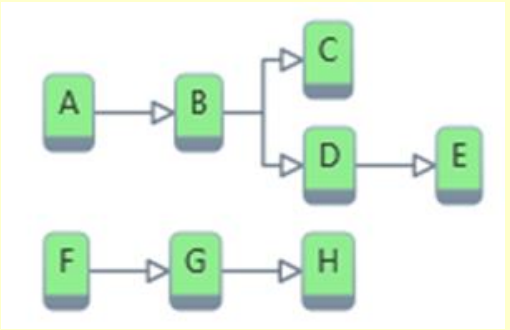
Kamal-Sourour

...

Friedman

Ozawa

...



Simulations

Predictions:
isothermal / dynamic / arbitrary

Predictions:
degree of cure / curing rate / viscosity

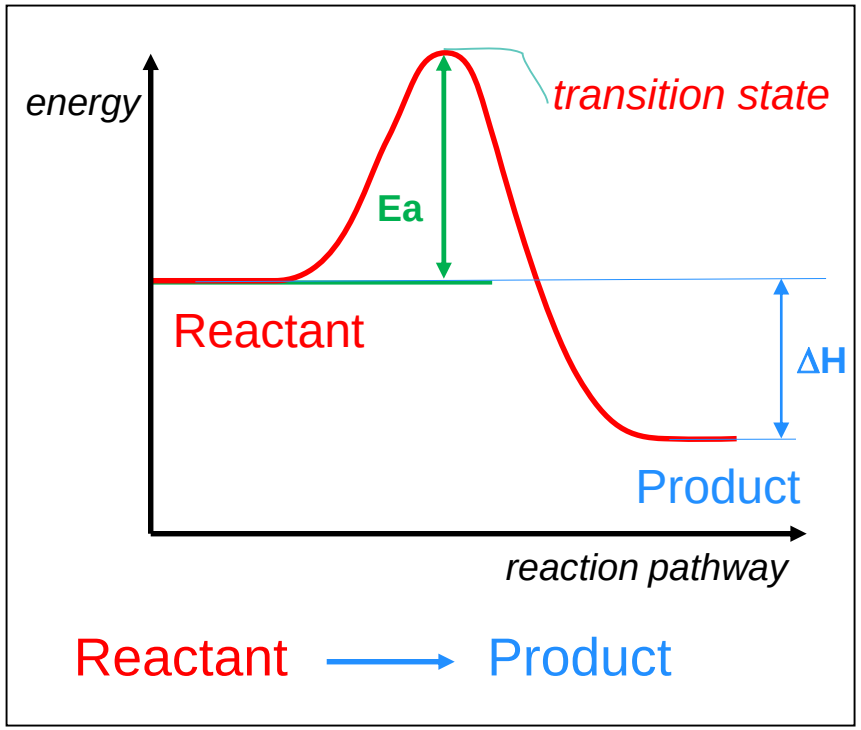
...

Optimization:
conversion rate

Optimization:
curing profile

...

2.2 Arrhenius equation. Activation energy. Kinetic triplet



Arrhenius equation (1889) for reaction rate:

$$\frac{d\alpha}{dt} = A\ exp\left(\frac{-E_A}{RT}\right)\ f(\alpha)$$

Conversion α: degree of conversion, changing from 0 to 1

Pre-exponent A: collision frequency [1/s]

Activation energy Ea [kJ/mol]

$f(\alpha)$ Reaction type (nth order, autocatalysis, nucleation …)

R: gas constant 8.31 [J/(gK)] T: absolute temperature [K] T[K]=T[°C]+273.15

2.3 Approaches: model free and model based

Model free

A → B

α – degree of conversion

$$\frac{d\alpha}{dt} = A(\alpha) \cdot f(\alpha) \cdot exp\left(\frac{-E_A(\alpha)}{RT}\right)$$

Unknown: Ea(α) and A(α)
A(α) can be found only with assumption of f(α)

Assumptions:

1. Only **one** kinetic equation
2. Ea and A **depend on α**
3. Reaction rate at the same conversion is only a function of temperature
4. Total effect (total mass loss or total peak area) must be the **same for all curves**
5. **Changes** of mechanism should be at the **same conversion** value

Model based

A → B → C → …

a – concentration of A
b – concentration of B
c – concentration of C

$$\frac{d(a \to b)}{dt} = A_1 \cdot f_1(a.b) \cdot exp\left(\frac{-E_{A1}}{RT}\right)$$

$$\frac{d(b \to c)}{dt} = A_2 \cdot f_2(b.c) \cdot exp\left(\frac{-E_{A2}}{RT}\right)$$

The number of unknown kinetic triplets equals the number of the steps

Assumptions:

1. Reaction consists of **several individual reaction steps** with own equations.
2. All kinetic parameters which are the **constant values**
3. The **total signal** is the **sum** of the signals of the single reaction steps having **own weight**

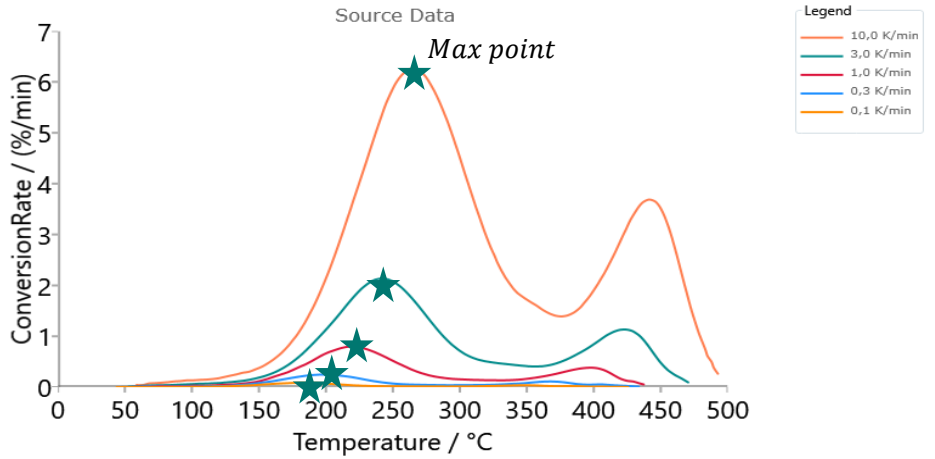
2.3 Model free methods in Kinetics Neo

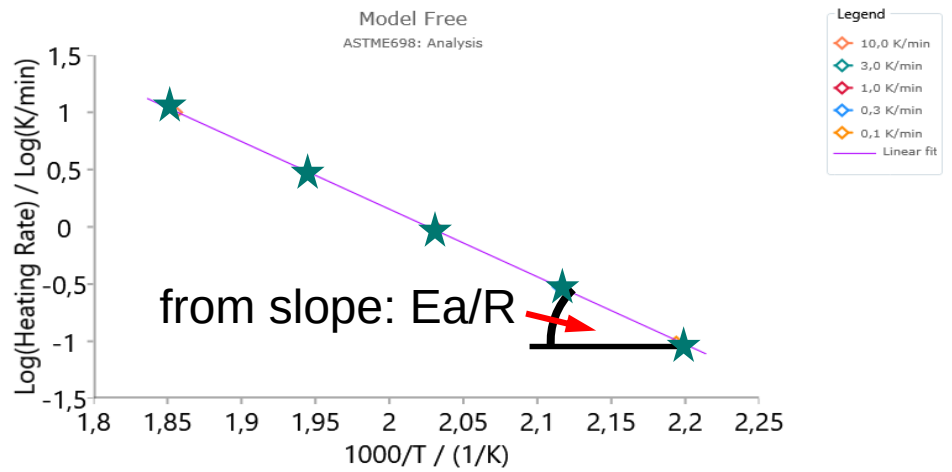
Created in last century before the modern possibilities of personal computers

One-point model free methods

- ASTM E698
- ASTM E2890
- ASTM E1641
- ASTM E2070

Result: **Value Ea**

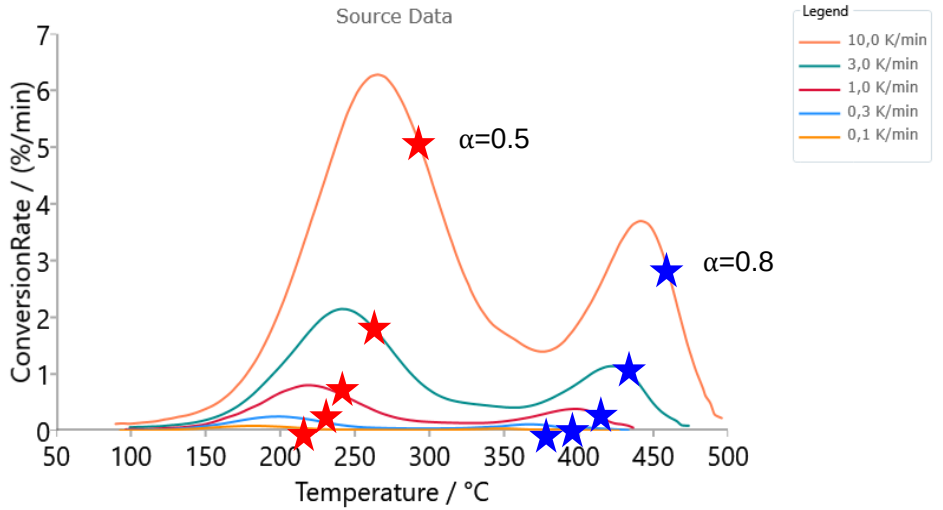


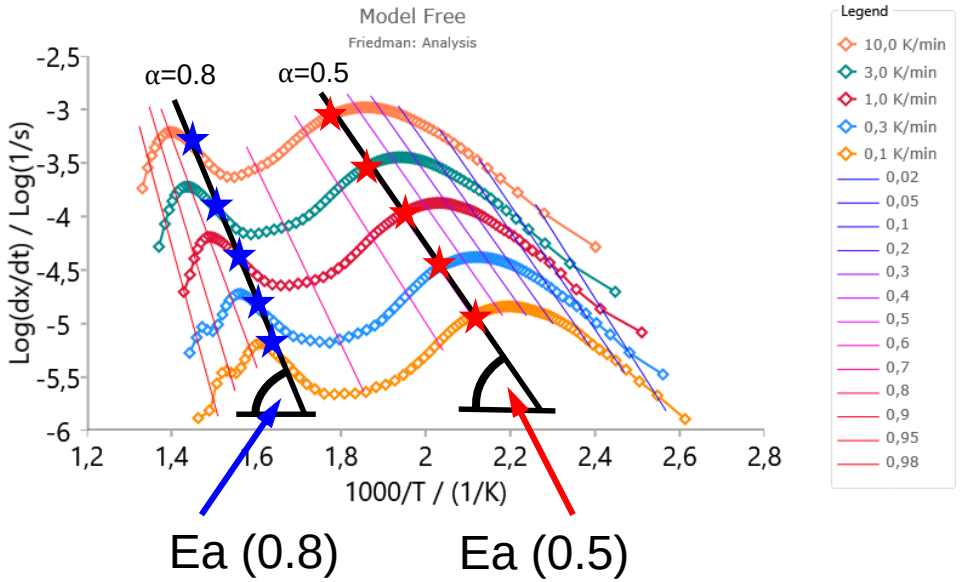


Multi-points model free methods

- Ozawa-Flynn-Wall (1965)
- Kissinger-Akahira-Sunose (1956)
- Friedman method (1966)
- Vyazovkin for heating (1996)
- Numerical optimization

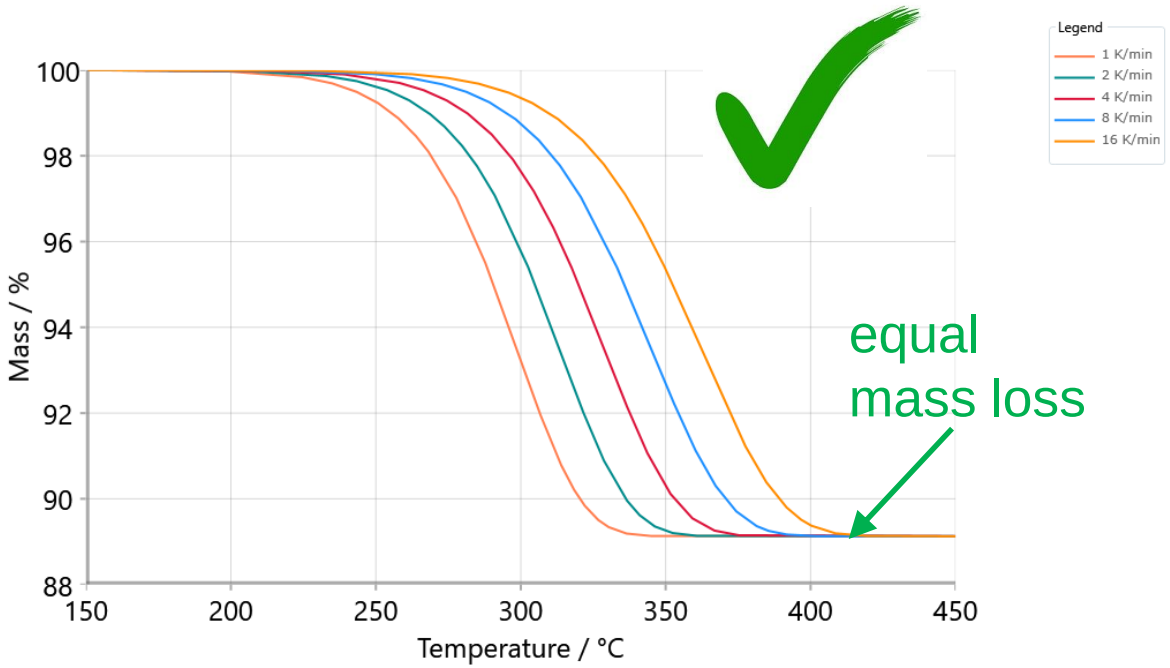
Result: **Function Ea(α)**

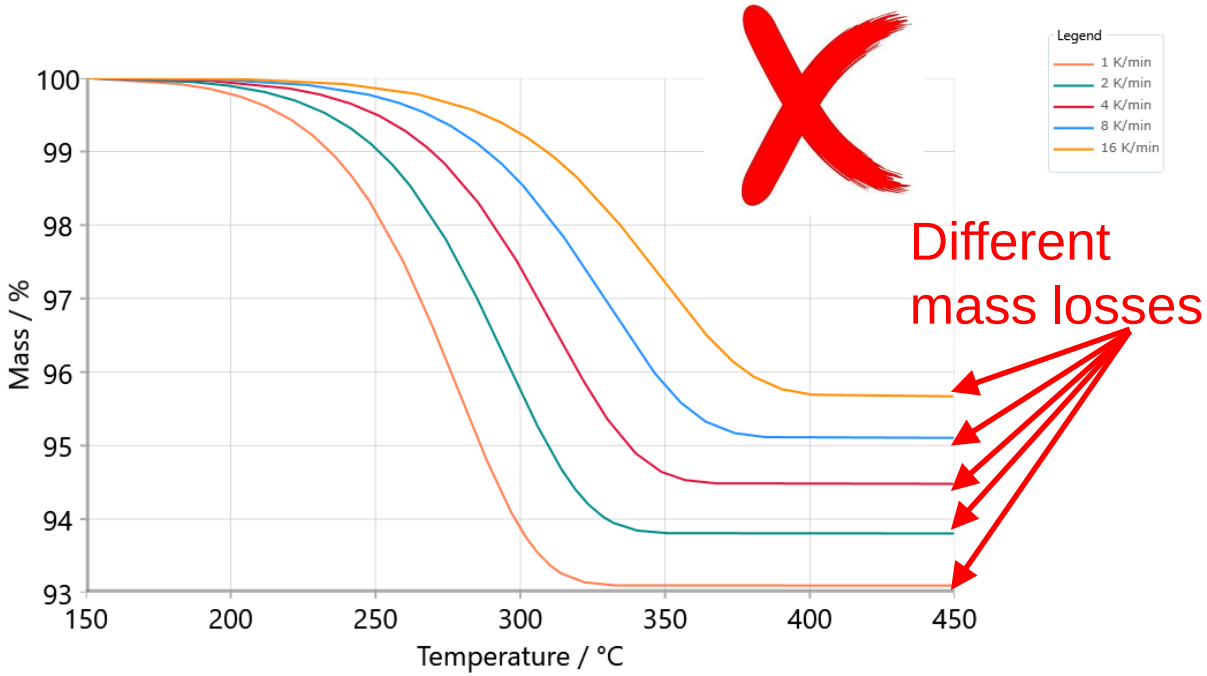




2.4 When model-free method is applicable

Total effect (total mass loss or total peak area) must be the same for all curves

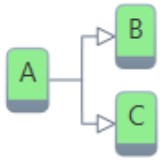




Model free is applicable

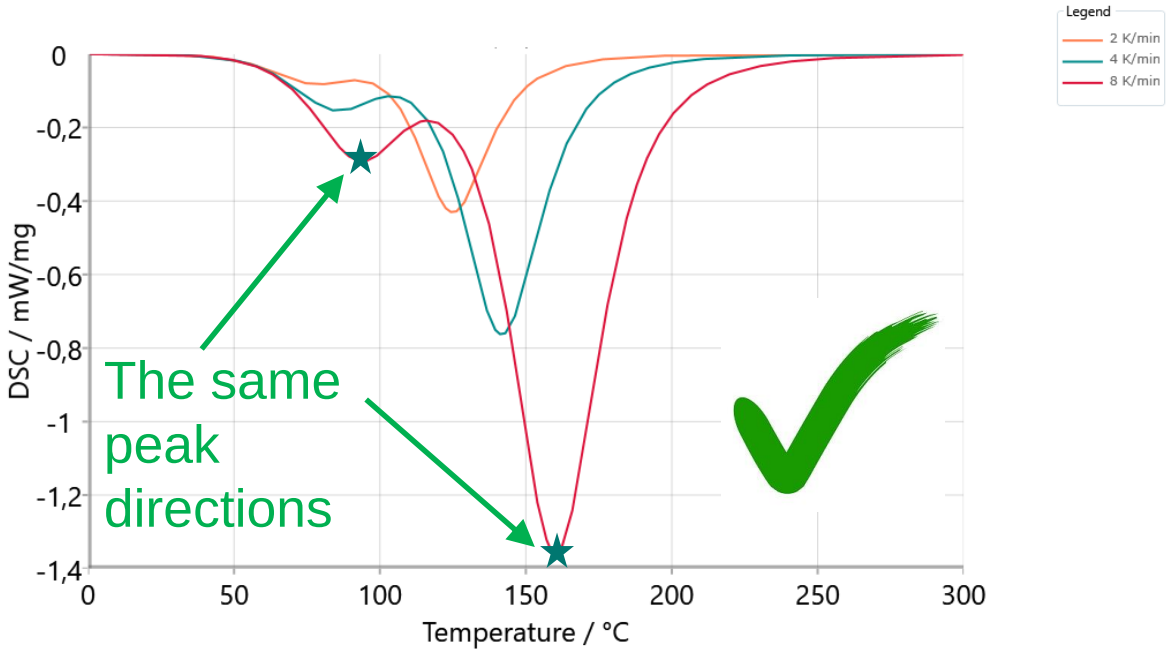
Model free is **not** applicable

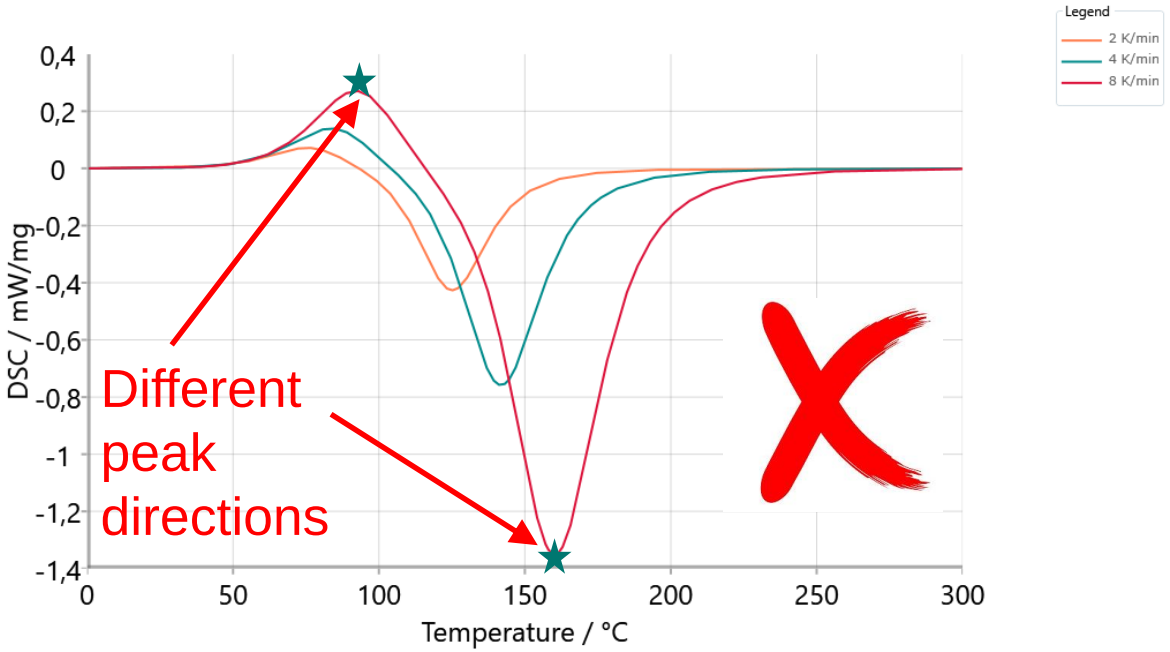
Solution: Model based method with competitive steps



2.4 When model-free method is applicable

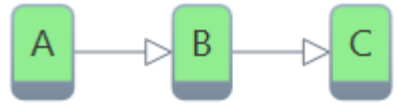
There is no reaction steps of different directions
(e.g. exothermal and endothermal, mass loss and mass gain)





Model free is applicable

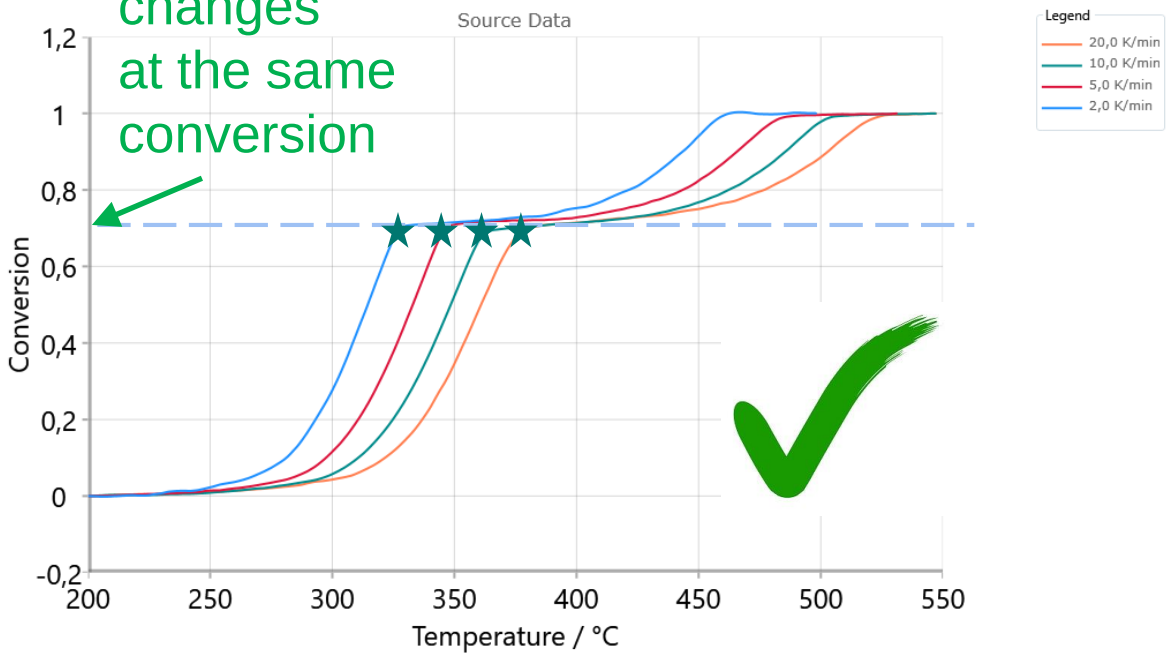
Model free is **not** applicable
Solution: Model based method
with steps contributions of different signs



2.4 When model-free method is applicable

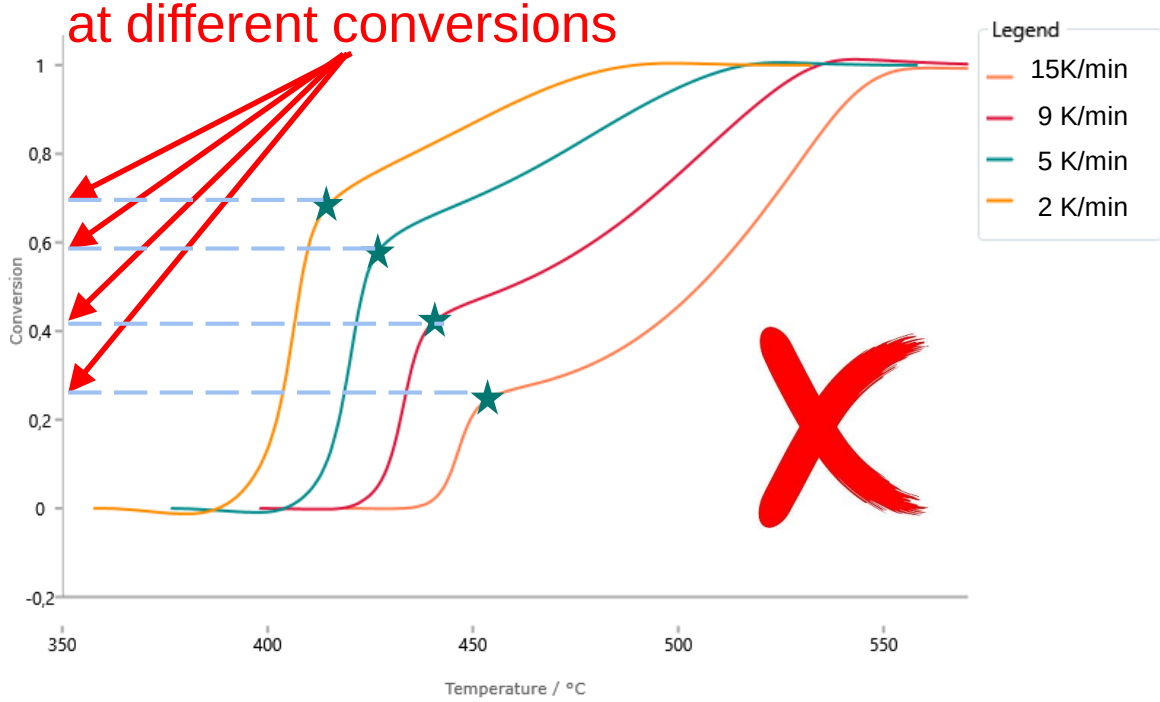
Changes of mechanism should be at the same conversion value

Mechanism changes at the same conversion



Model free is applicable

Mechanism changes at different conversions



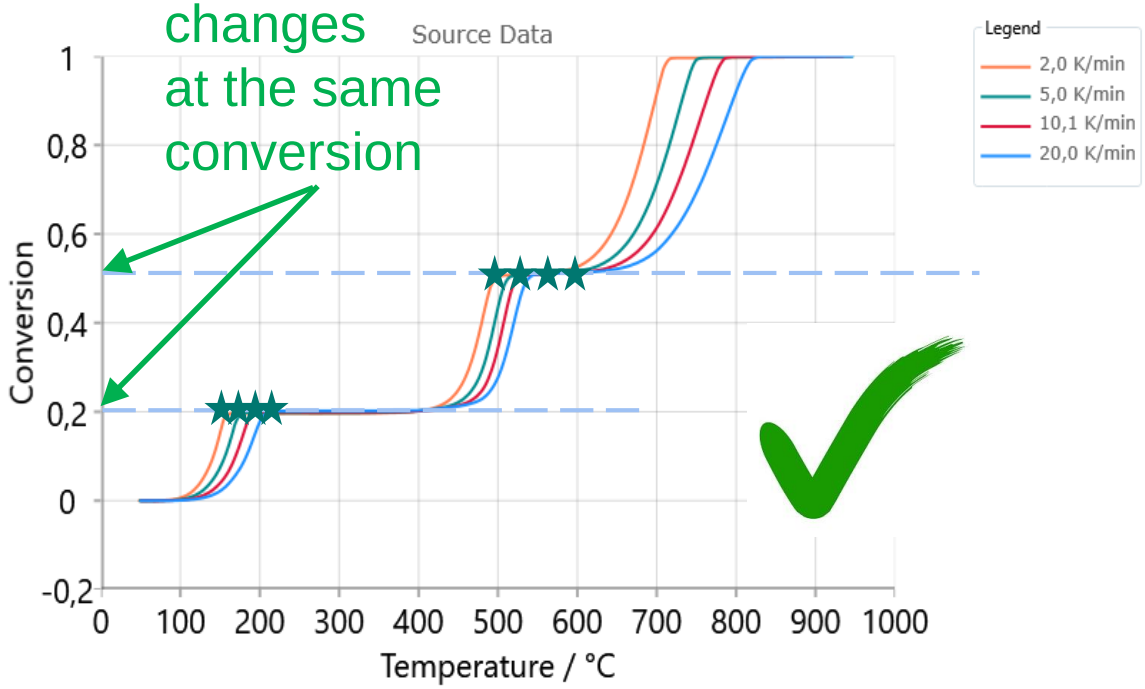
Model free is **not** applicable

Solution: Model based method with competitive steps

2.4 When model-free method is applicable

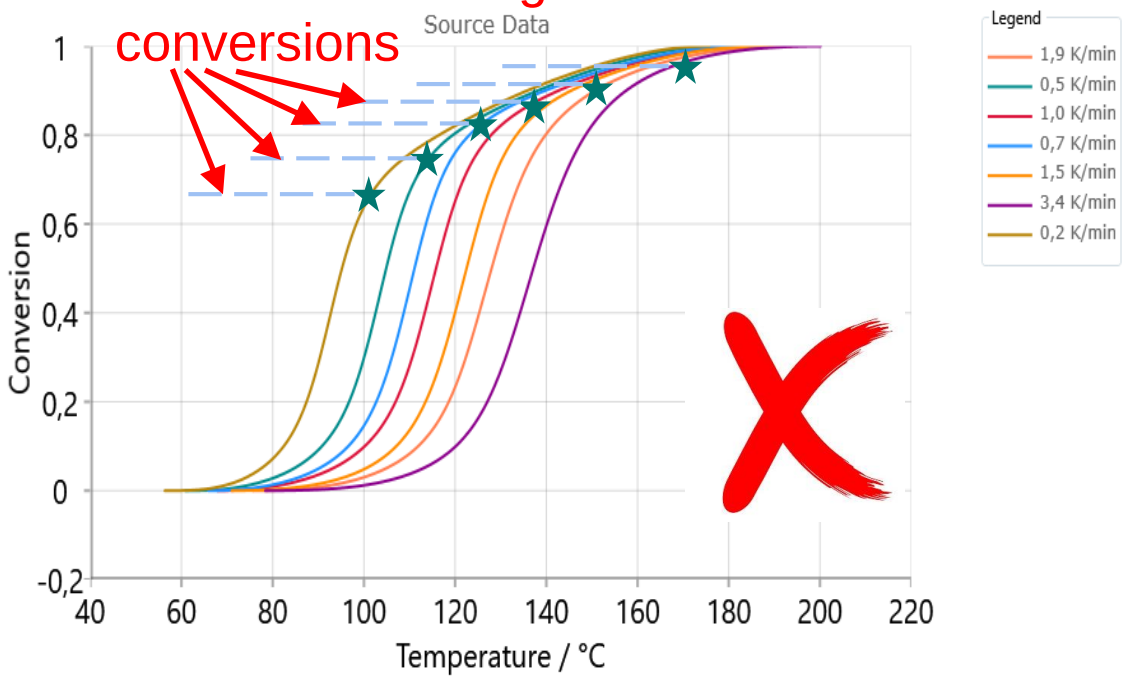
Changes of mechanism should be at the same conversion value

Mechanism changes at the same conversion



Model free is applicable

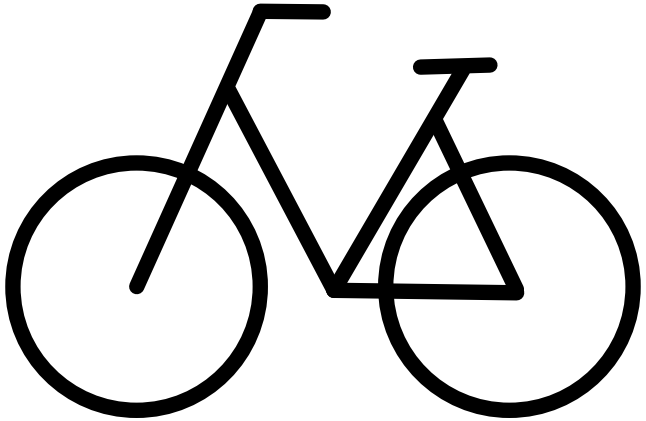
Reaction with diffusion control: mechanism changes at different conversions



Model free is **not** applicable

Solution: Model based method with diffusion control

2.5 Advantages and disadvantages



2.5 Advantages and disadvantages

Model free

Advantages:

1. Very fast, one click
2. Easy analytical methods, mostly can be done in Excel

Disadvantages:

1. Does not work for **mixtures** (independent parallel steps)
2. Does not work for **competitive steps**
3. Does not work for **curing with Kamal Sourour** reaction
4. Does not work for **curing with diffusion control**
5. Does not work for **crystallization**
6. Does not work for **the steps of different directions**
7. Does not work for **highly overlapping steps**
8. Does not work if **reaction mechanism changes with heating rate**
9. Has **no** any information about **intermediate steps** and reactants

Model based

Advantages:

1. Works for **mixtures** (independent parallel steps)
2. Works for **competitive steps**
3. Works for **curing with Kamal Sourour** reaction
4. Works for **curing with diffusion control**
5. Works for **crystallization**
6. Works for **the steps of different directions**
7. Works for **highly overlapping steps**
8. Works if **reaction mechanism changes with heating rate**
9. Has information about **intermediate steps** and reactants

Disadvantages:

1. Requires elementary chemical knowledge about the process
2. Number of steps usually should not exceed the number of visible peaks

It is necessary to use ICTAC kinetic recommendations

https://doi.org/10.1016/j.tca.2020.178597

3. Unique features of Kinetics Neo software

3.1 Fulfils all ICTAC kinetic recommendations
3.2 Numerical model free method
3.3 Special functions for curing (Kamal-Sourour, Diffusion control, TTT diagram, viscosity prediction)
3.4 Crystallization kinetics
3.5 Multi-step model based method, including presentation of each individual reaction step
3.6 Small other features (Bezier baseline, export equations…)

All Kinetics Neo features: https://kinetics.netzsch.com/en/docs

Technical Datasheet: **Kinetics Neo 2.5**
kinetics.netzsch.com

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Model-Free Methods	
Definition	Model-free analysis allows to find the activation energy of the reaction without assumption of a kinetic model for it.
Methods based on a single conversion	• ASTM E698 • ASTM E2890 • ASTM 1641 • Isothermal Arrhenius for time-to-event • Dynamic Arrhenius for failure temperature
Conversion-dependent methods	• Friedman • Ozawa-Flynn-Wall (OFW) • Kissinger-Akahari-Sunose (KAS) • ASTM E2070(A) for isothermal data • Vyazovkin for dynamic data • Numerical Optimization The numerical model-free method ensures fast determination of the best model-free solution to achieve best the agreement between simulated and experimental curves
Results	• Analysis graph • Plot of activation energy vs degree of conversion • Plot of pre-exponential factor vs degree of conversion • Master plot f(α) • Conversion fit for signal, conversion and conversion rate

Model-Based Methods	
Multi-step analyzing engine	Model-free methods allow for analyzing only one-step kinetic processes. However, approximately 95% of all chemical reactions are multi-step reactions. This requires the multi-step analyzing engine of the Kinetics Neo software.
Unique features	The model-based kinetic analysis is based on an unlimited number of models including an unlimited number of reaction steps where the individual steps are linked as independent, parallel, competing or following.
Kinetic models	Visual creation of a kinetic model. Visual adding, removing or editing of each reaction step. Visual adjustment of position, contribution, activation energy and peak shape of each step. Optimization of kinetic parameters for one individual step. Optimization of kinetic parameters for the complete kinetic model.
Reaction types	Each individual reaction step in each model can be one of 19 reaction types including • Reaction of 1st, 2nd and n-th order without autocatalysis • Reaction of 1st, 2nd and n-th order without autocatalysis including Prout-Tompkins and Kamal-Sourour reactions • 2-/3-dimensional phase boundary reactions • 1-/2-/3-dimensional diffusion (Jander's type and Ginstling-Brounstein) • Prout-Tompkings reaction • 2-/3-/n-dimensional nucleation according to Avrami • Reactions with diffusion control • Crystallization according to the Nakamura equation using the Hoffman-Lauritzen Theory **Models for glass transition function for diffusion control** • Di Benedetto model • Splines
Kinetic results	The software determines the kinetics model including • Number of reaction steps • Step contribution to the total effect **Standard parameters for each reaction step:** • Reaction type • Activation energy • Reaction order **Additional parameters for some reaction types** • Order of autocatalysis • Dimension of nucleation or diffusion **Parameter for crystallization** • Dimension of nucleation • Melting temperature and glass transition temperature • Nakamura parameter K_G
Stastical results	• Correlation coefficient • Sum of the squares of deviations • Mean residual • t-value • Durbin-Watson value • Durbin-Watson test • F-test for fit quality • F-test for the number of steps

2|4

Technical Datasheet: **Kinetics Neo 2.5**
kinetics.netzsch.com

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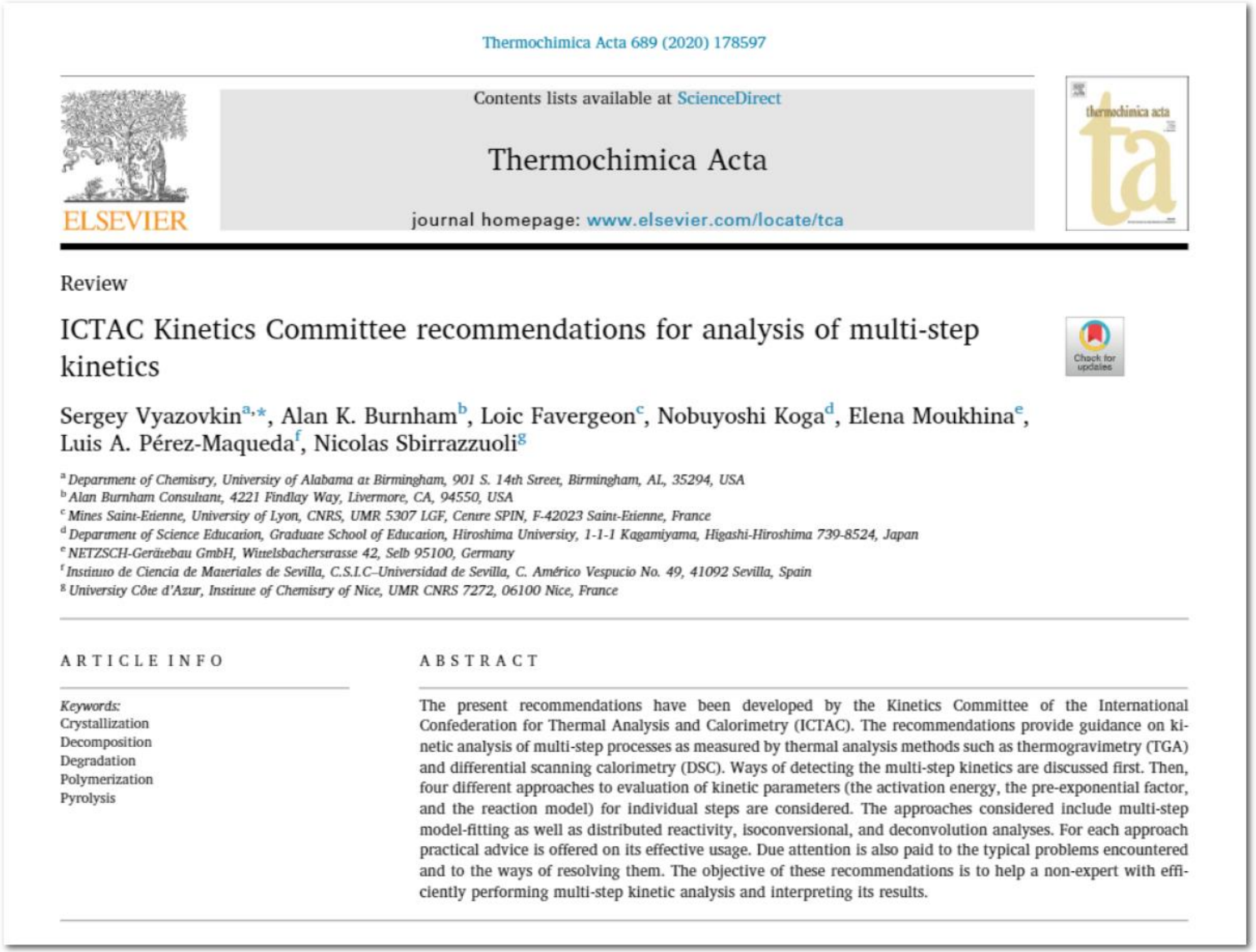
Predictions	
Isothermal predictions	Predictions for several isothermal temperatures
Isothermal lifetime predictions	Predictions for given conversion at several isothermal temperatures
Dynamic prediction	Predictions for several heating rates for reactions or for several cooling rates for crystallization
Multi-step prediction	Prediction for a user-defined sequence of dynamic and isothermal segments with the possibility of export/import of multi-step program to/from text file
Step-iso prediction	Prediction of a step-iso temperature program, representing a stepwise temperature increase
Modulated predictions	Prediction of a modulated temperature program which is the sum of an underlying constant temperature or constant heating and a sinus-shaped temperature oscillation
Adiabatic prediction	Calculation of the adiabatic temperature increase for various initial temperatures.
Adiabatic 24 (TD24)	Find the start temperature for adiabatic process at maximum heating rate in 24 hours
Climatic prediction	Prediction for the real atmospheric temperatures for a selected point on the Earth, from the selected day of the year, for the selected durations, which is usually several months or years.
Predictions based on external temperature profile	Prediction for temperature program loaded from external text file (ASCII of CSV) which includes time and temperature columns
Prediction unter pre-defined fire conditions	This method uses standard fire presets loaded into external temperature profile prediciton
TTT diagram	Time-Temperature-Transition diagram for reactions with diffusion control.
Results of prediction according to the user-defined temperature program	After input of the temperature program by the user, the software will make a simulation of the system behavior. The following values can be simulated: • Measurement output (signal) • Conversion • Conversion rate • Concentration of the reactants for model-based method only • Reaction rate for individual reaction steps for model-based method only • Presentation of conversion rate as the sum of individual reaction steps • Predictions of raw viscosity for viscosity project type The simulated values can be presented: • Curves as a function of time • Curves as a function of temperature • Table with simulated values, time and temperature

Optimization	
Conditions for optimization	Finding a temperature program for a given system behavior (optimization). It is the typcial question arising during a production process. The temperature program for optimal time and quality must be found. Without the Kinetics Neo software, it is necessary to make an adjustment of the temperature program by hand and to measure several times while hoping to achieve the expected signal curve. The software – in contrast – saves time and finds such a temperature program • For a given reaction rate • For a given output signal • For a given rate of the final product production • For user-defined function of conversion versus time
Results of optimization	• Temperature program • Measurement output (signal) • Conversion • Conversion rate • Concentration of the reactants, for model-based method only • Reaction rate for individual reaction steps, for model-based method only • Presentation of conversion rate as the sum of individual reaction steps • Prediction of raw viscosity for viscosity project type • Sum of peaks presents the total conversion-rate curve as the sum of the individual reaction peaks The simulated values can be presented: • Curves as a function of time • Curves as a function of temperature • Table with simulated values, time and temperature

3|4

3.1 Unique: Kinetics Neo fulfils ICTAC kinetics recommendations

International Confederation for Thermal Analysis and Calorimetry



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Review

ICTAC Kinetics Committee recommendations for analysis of multi-step kinetics

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ARTICLE INFO

Keywords:
Crystallization
Decomposition
Degradation
Polymerization
Pyrolysis

ABSTRACT

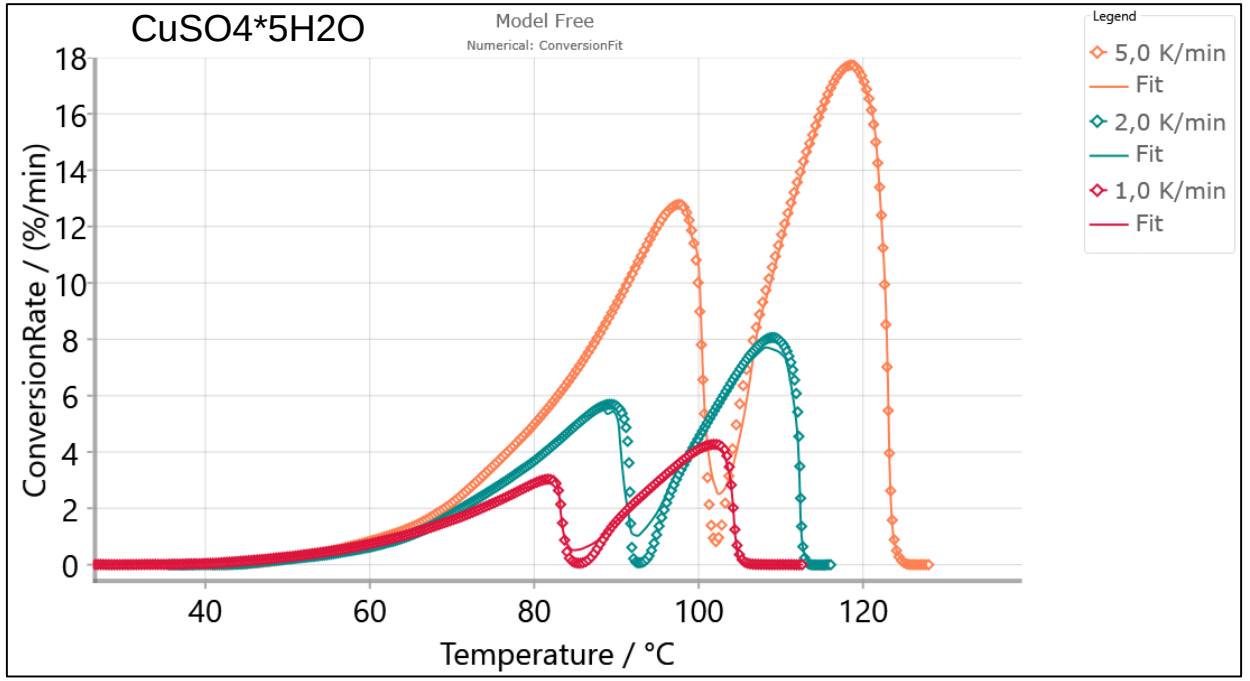
The present recommendations have been developed by the Kinetics Committee of the International Confederation for Thermal Analysis and Calorimetry (ICTAC). The recommendations provide guidance on kinetic analysis of multi-step processes as measured by thermal analysis methods such as thermogravimetry (TGA) and differential scanning calorimetry (DSC). Ways of detecting the multi-step kinetics are discussed first. Then, four different approaches to evaluation of kinetic parameters (the activation energy, the pre-exponential factor, and the reaction model) for individual steps are considered. The approaches considered include multi-step model-fitting as well as distributed reactivity, isoconversional, and deconvolution analyses. For each approach practical advice is offered on its effective usage. Due attention is also paid to the typical problems encountered and to the ways of resolving them. The objective of these recommendations is to help a non-expert with efficiently performing multi-step kinetic analysis and interpreting its results.

KINETICS NEO

- Model free analysis
- Multi-step model-fitting (model based)
- Diffusion control for curing
- Crystallization kinetics
- Kamal model for curing
- Deconvolution analysis (sum of peaks)
- ~~Distributed reactivity analysis~~

3.2 Unique: Model-free methods, Numerical method

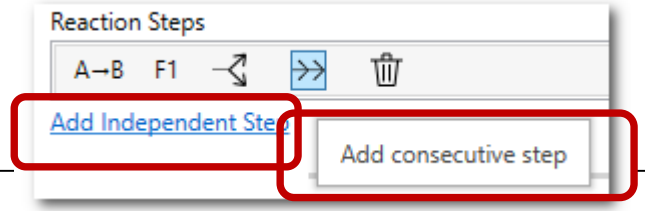
- **Model-Free**
  - ASTM E698
  - ASTM E2890
  - ASTM E1641
  - Dynamic Arrhenius
  - Isothermal Arrhenius
  - ASTM E2070
  - Friedman
  - Ozawa-Flynn-Wall
  - Kissinger-Akahira-Sunose
  - Vyazovkin
  - Numerical Optimization

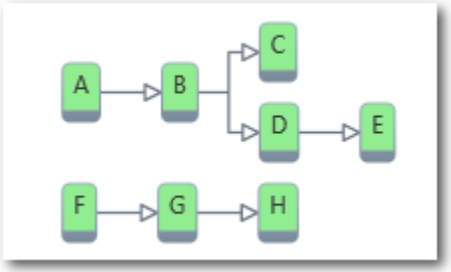


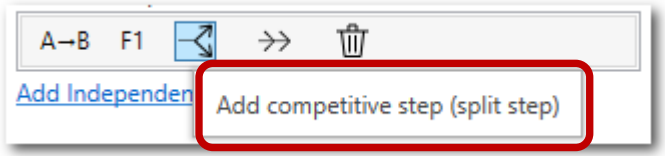
Please always check the fit visually

Method/Model	Fit To	R^2	Sum of dev. squares	Mean Residual
Numerical	Signal	0,99655	2,092	0,023
Friedman	Signal	0,99237	4,612	0,030
Vyazovkin	Signal	0,97562	14,611	0,054
KissingerAkahiraSunose	Signal	0,87774	69,648	0,138
OzawaFlynnWall	Signal	0,85547	81,358	0,165
ASTME1641	Signal	0,71256	149,337	0,205
ASTME2890	Signal	0,70314	153,383	0,264
ASTME698	Signal	0,70182	153,947	0,264

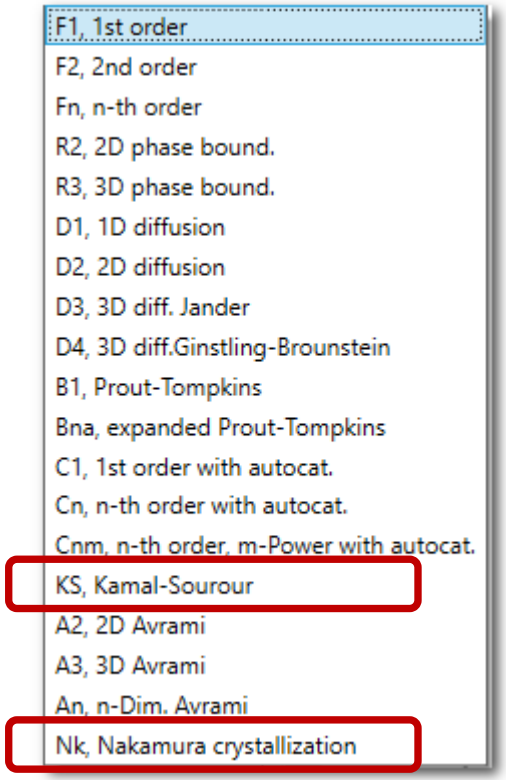
3.3 Unique: Model based analysis







- Modelling
  - unlimited number of models
  - unlimited number of reaction steps
  - individual steps are linked as independently, parallel, competing or following
  - Visual creation of a kinetic model
  - Visual adding, removing or editing of each reaction step.
  - Optimization of kinetic parameters for one individual step.
  - Optimization of kinetic parameters for the complete kinetic model.



- Reaction types
  - Reaction of 1st, 2nd and n-th order without autocatalysis
  - Reaction of 1st, 2nd and n-th order with autocatalysis including Prout-Tompkins and Kamal-Sourour reactions
  - 2-/3-dim. phase boundary reactions
  - 1-/2-/3-dim. diffusion (Jander's type and Ginstling-Brounstein)
  - 2-/3-/n-dim. nucleation according to Avrami
  - Curing Reactions with diffusion control (using DiBenedetto model or splines for dependence Tg vs Alpha)
  - Crystallization according to the Nakamura equation using the Hoffman-Lauritzen theory

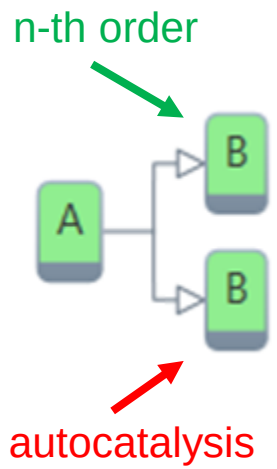
3.3.1 Unique: Kinetic Modelling for Curing

Chemical process is **generally** described by Arrhenius equation:

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot exp\left(\frac{-Ea}{RT}\right)$$

Curing can be described by the equation **Kamal-Sourour** for autocatalytic reaction:

$$\frac{d\alpha}{dt} = \underbrace{A \cdot (1-\alpha)^n \cdot \exp\left(\frac{-E_{a1}}{RT}\right)}_{\text{n-th order}} + \underbrace{A \cdot K \cdot (1-\alpha)^n \cdot \alpha^m \cdot \exp\left(\frac{-E_{a2}}{RT}\right)}_{\text{autocatalysis}}$$

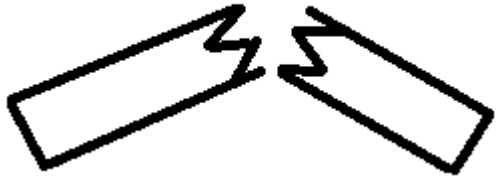


This **equation** with its parameters A, E_{a1}, E_{a2} , K, m, n, is the **kinetic model**.

Kinetic parameters are found from the **best fit** for all experimental data

Reaction finished

Cold



Glassy state

Warm

Rubbery or liquid state

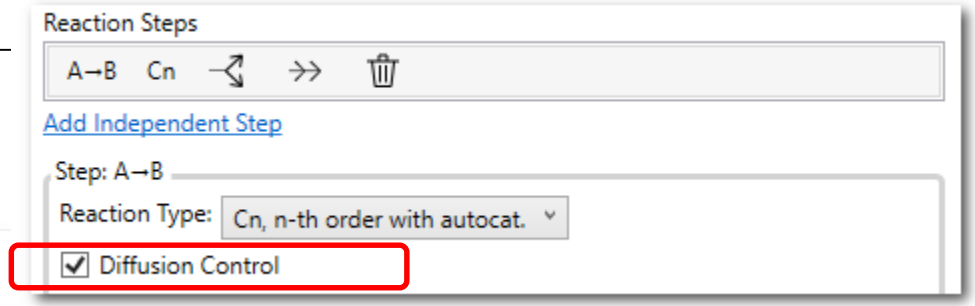
Tg

Slow curing
T<Tg

Fast curing
T>Tg

Glass transition

3.3.2 Unique: Experiment and Model Fit for diffusion control



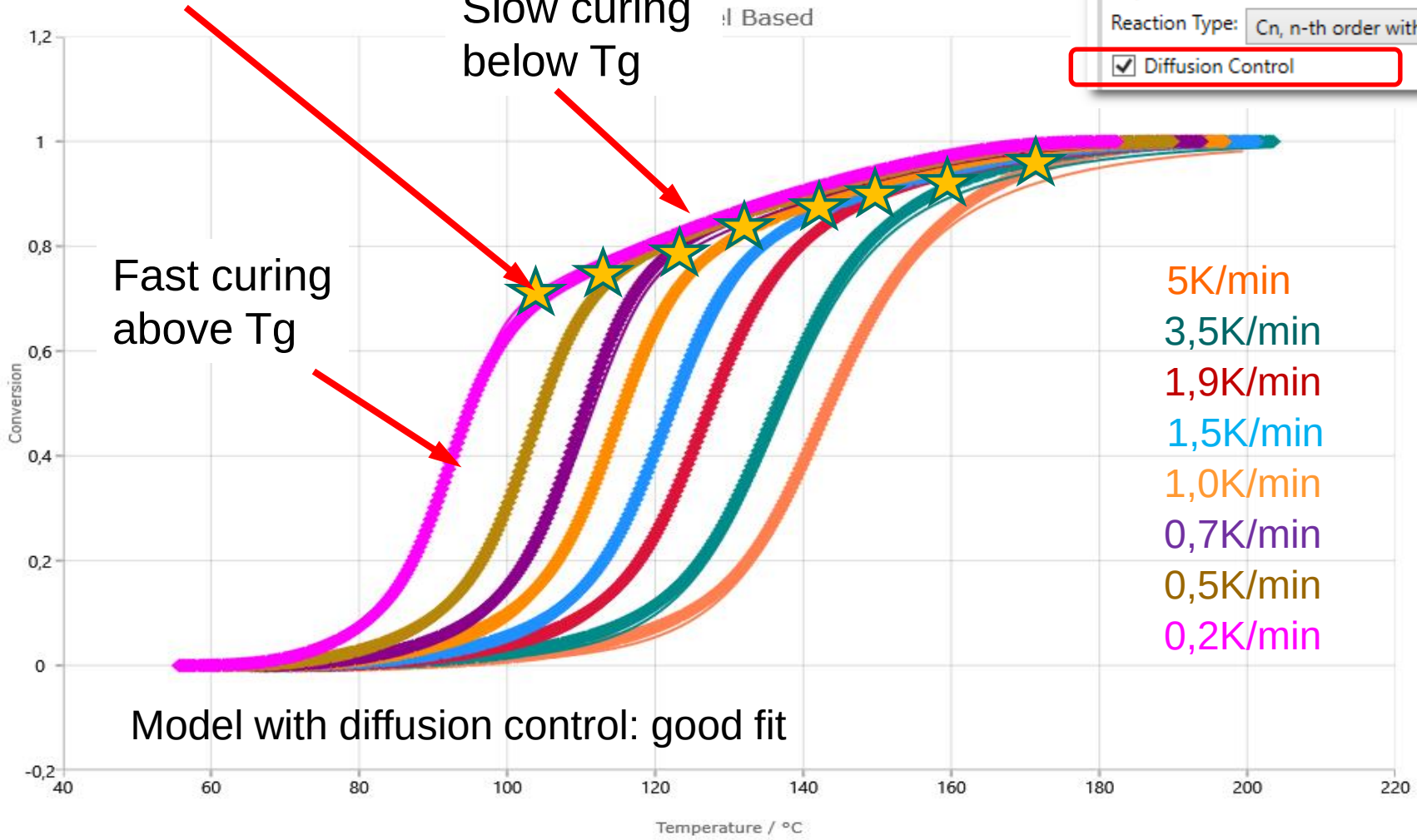
T=Tg, vitrification

Slow curing below Tg

Fast curing above Tg

5K/min
3,5K/min
1,9K/min
1,5K/min
1,0K/min
0,7K/min
0,5K/min
0,2K/min

Model with diffusion control: good fit



See Theory of diffusion control in
S.Vyazovkin, A.K.Burnham, L.Favergeon, N.Koga, E.Moukhina, L.A.Perez-Maqueda, N. Sbirrazuoli.
Thermochimica Acta 689 (2020) 1785977, ICTAC Kinetics Committee recommendations for analysis of multi-step kinetics

3.3.2 Unique: Isothermal Predictions of glass transition for Time-Temperature-Transition diagram

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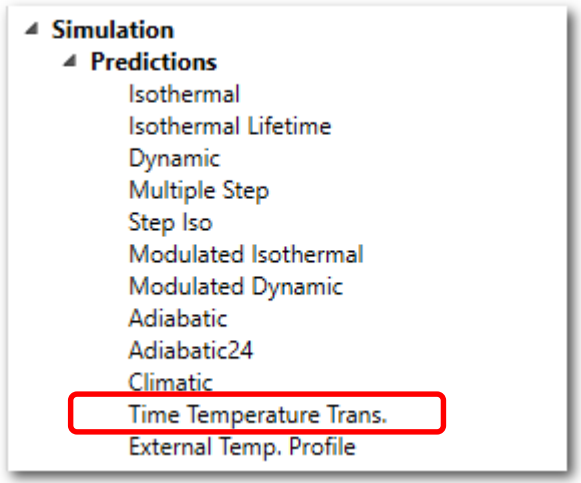
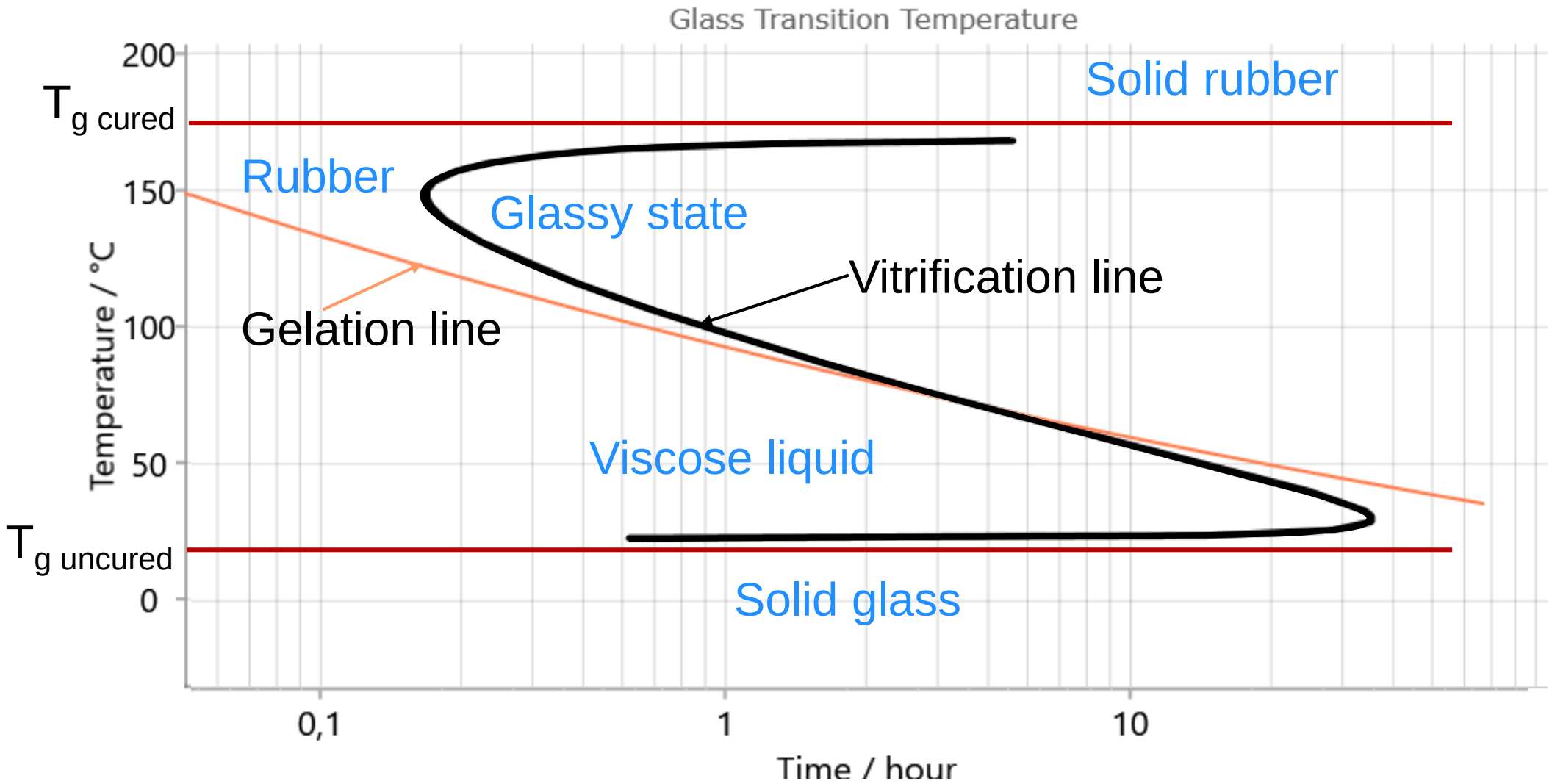
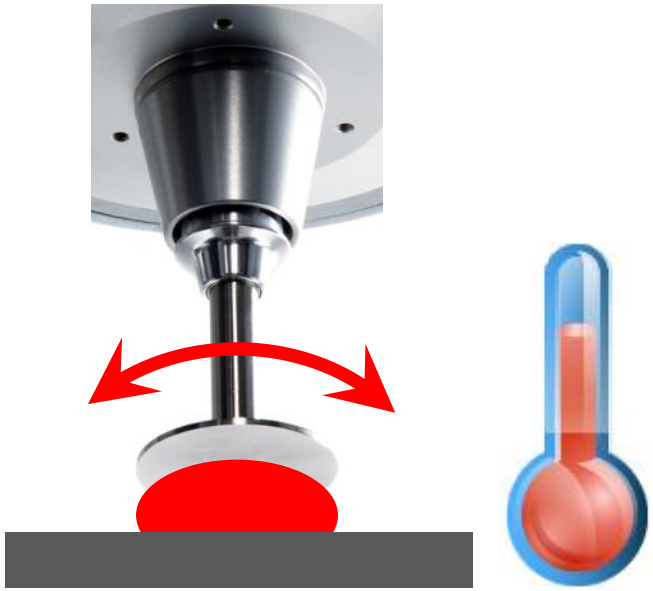


3.3.2 Unique: Time-Temperature-Transition diagram for curing



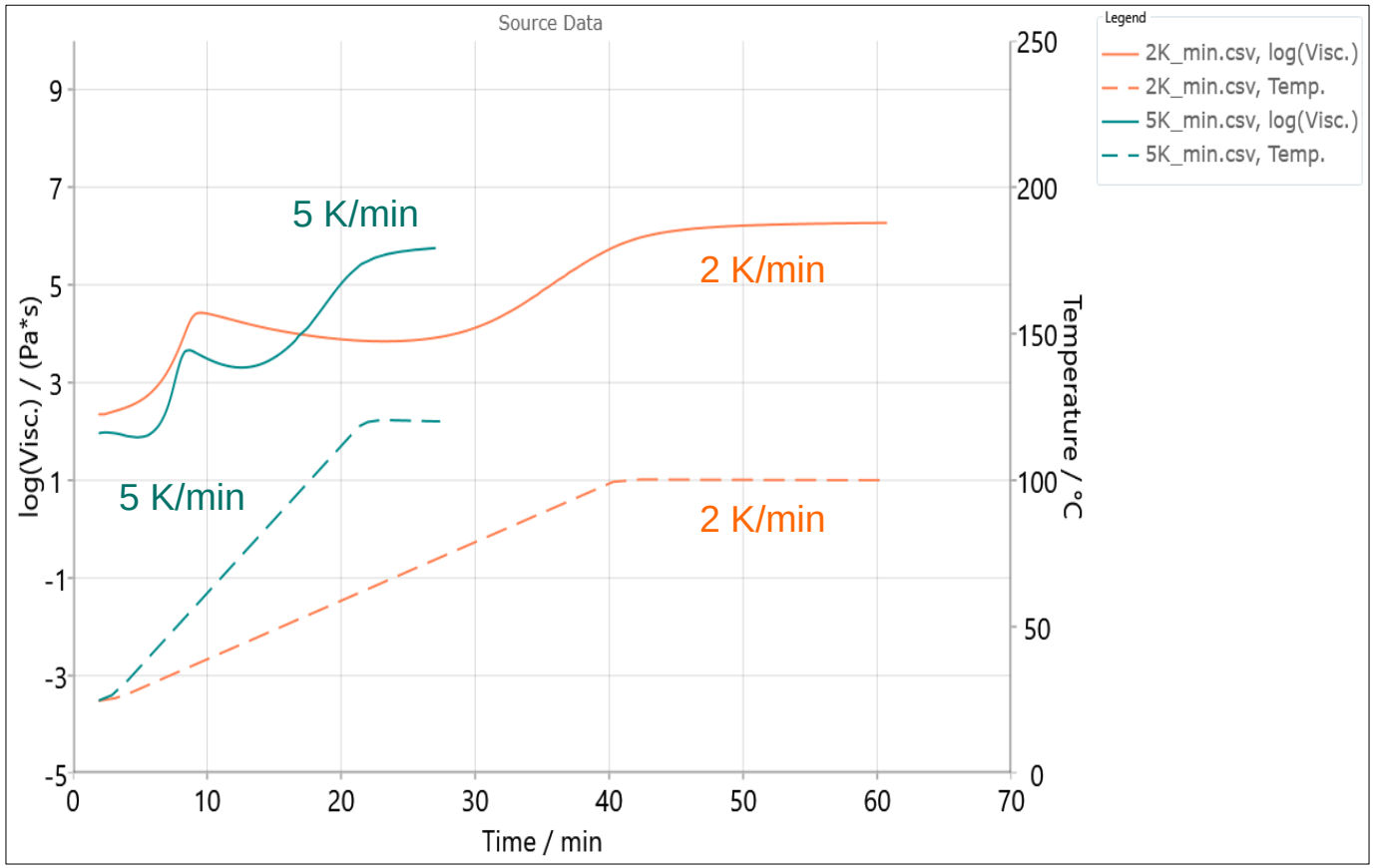
TTT Diagram shows the state of the material (glass, liquid, rubber) for isothermal conditions with known temperature and time

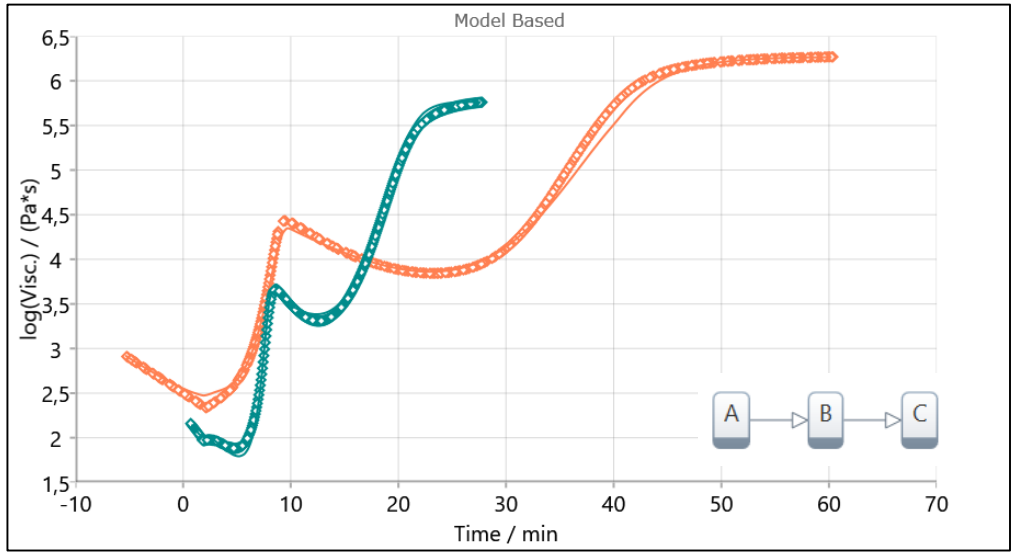
3.3.3 Unique: Kinetic analysis of rheological data and prediction of dynamic viscosity

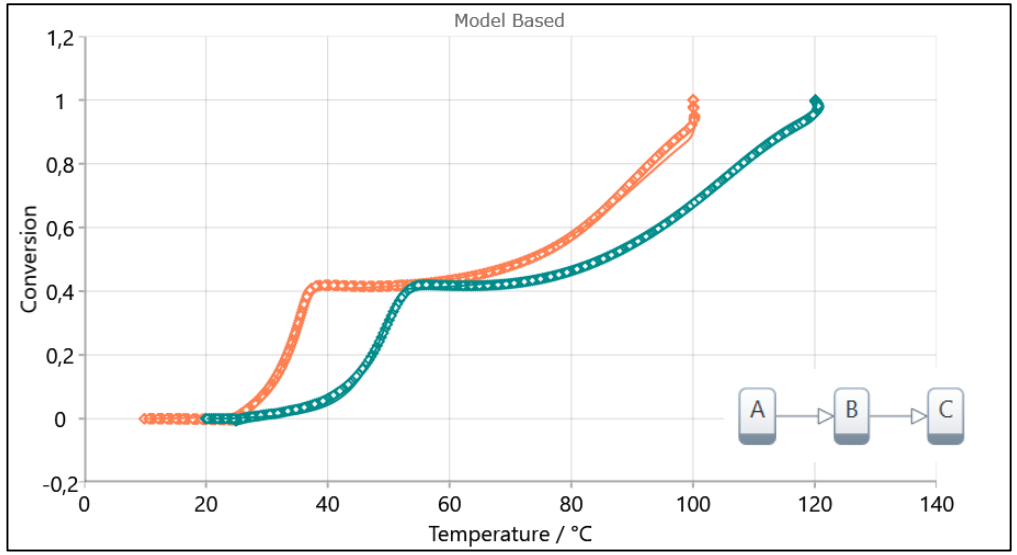


2-component adhesive
“Very fast setting”: 5 minutes…
Complete curing 24 hours

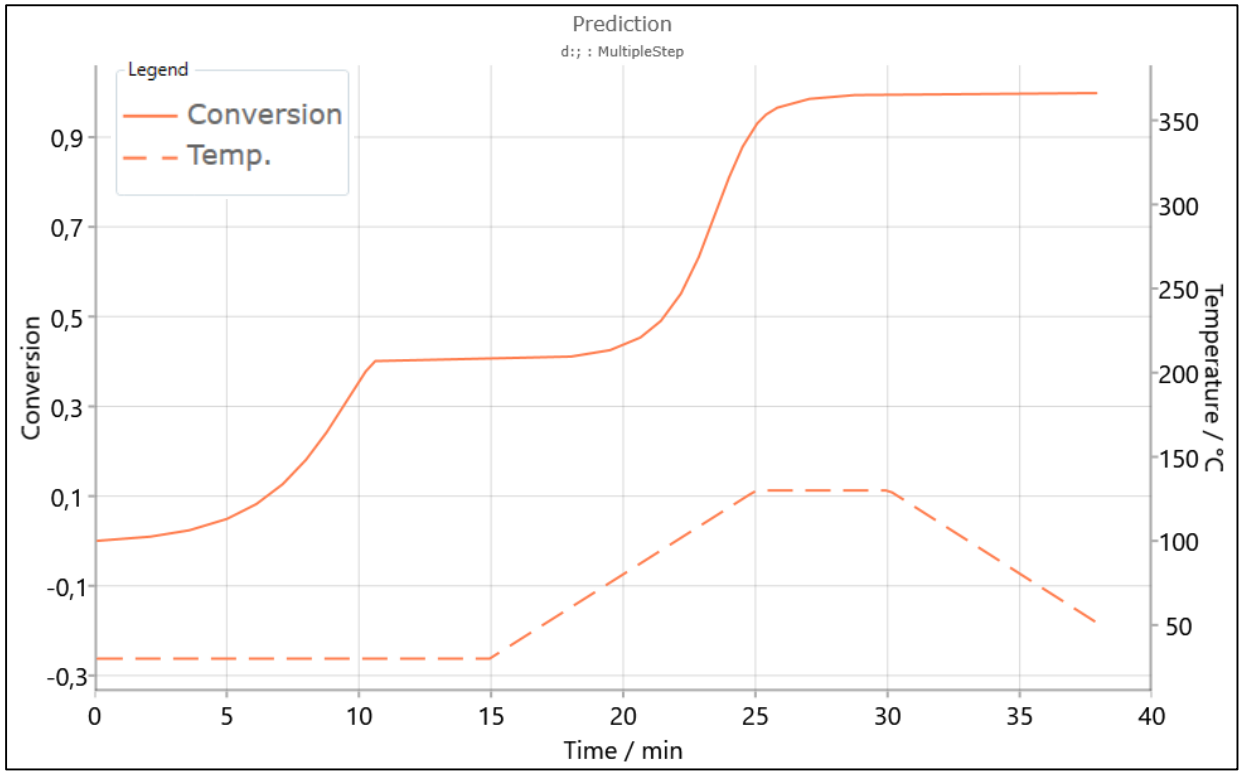
3.3.3 ARALDITE, Rheometry measurements for kinetic analysis

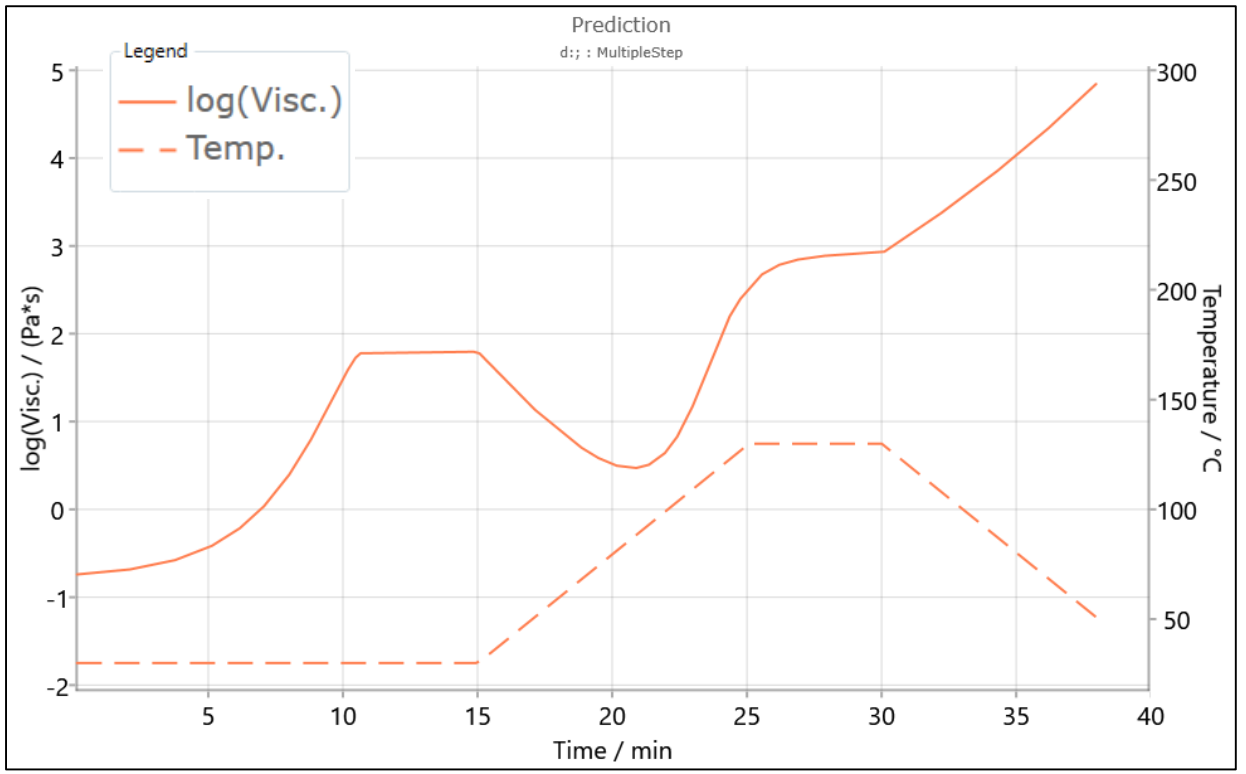






3.3.3 Prediction of conversion and viscosity for complex temperature program





3.4 Unique: Crystallization kinetics: non-Arrhenius approach: Nakamura und Hoffman-Lauritzen

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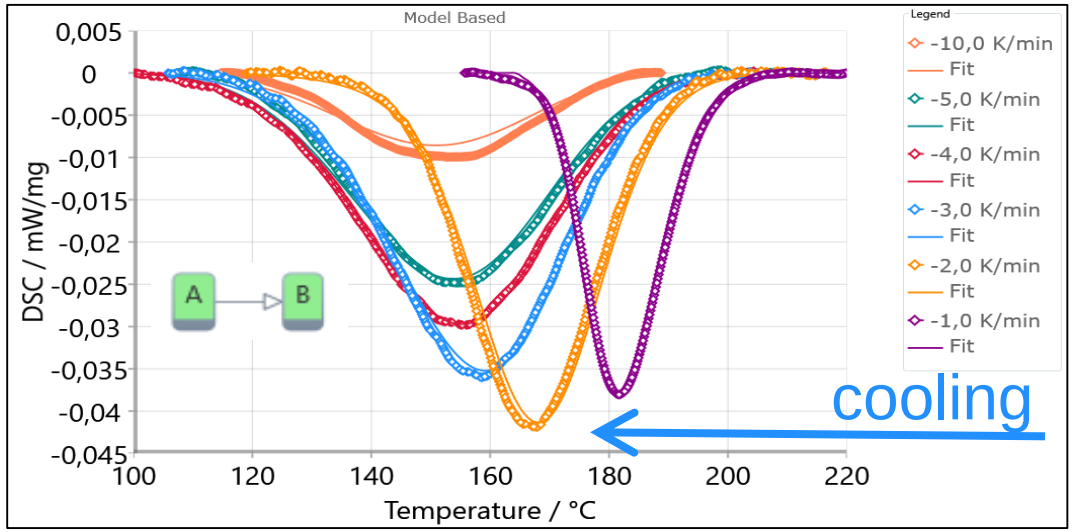
Avrami nucleation

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

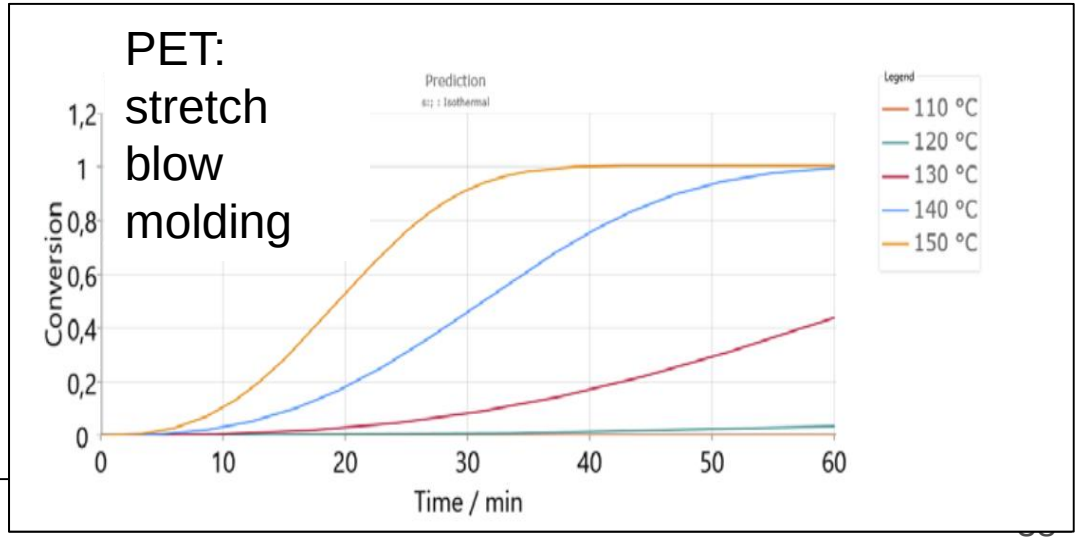
$$K(T) = exp\left(\frac{-U^*}{R(T - T_\infty)}\right) \cdot exp\left(\frac{-K_G}{T \cdot \Delta T \cdot f}\right)$$

U*	activation energy of segmental jump in polymers, this parameter has universal value 6.3kJ/mol
K_G	kinetic parameter for nucleation
ΔT=Tm-T	undercooling from the equilibrium ***melting point Tm***
T_∞=Tg-30	temperature at which crystallization transport is finished, this temperature is 30K below the ***glass transition temperature Tg***.
f=2T/(T+Tm)	correction factor

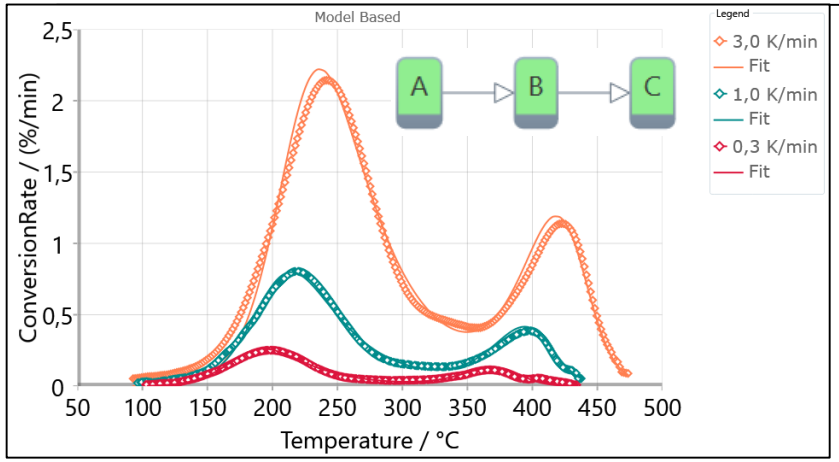
Measurement and Model for PET:



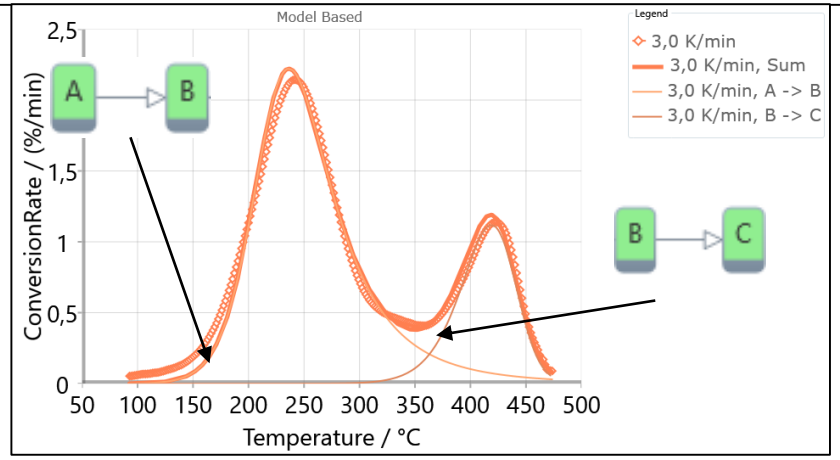
Predictions: Conversion



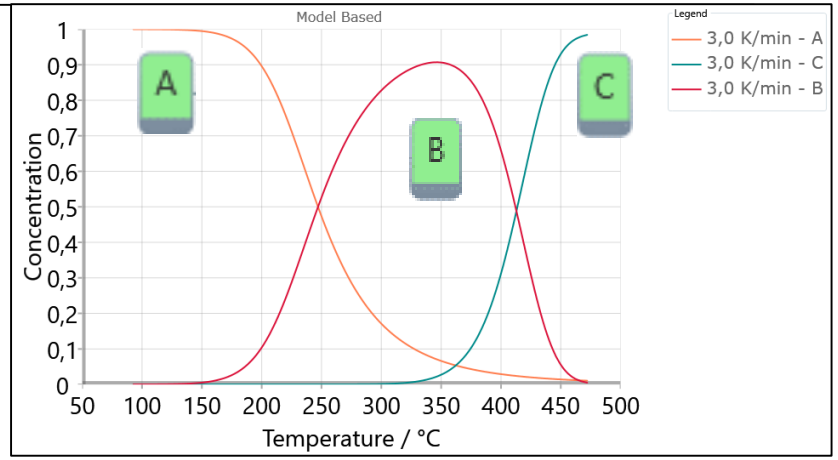
3.5 Unique: Model based method with reaction steps and concentrations



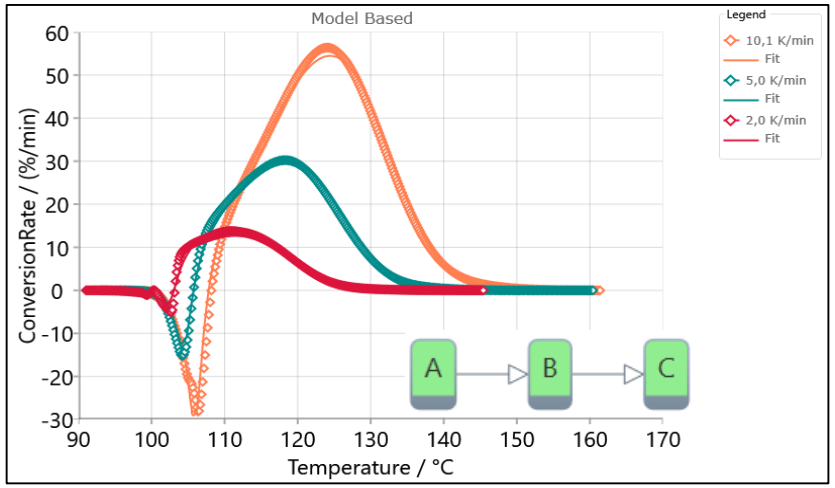
Kinetic model

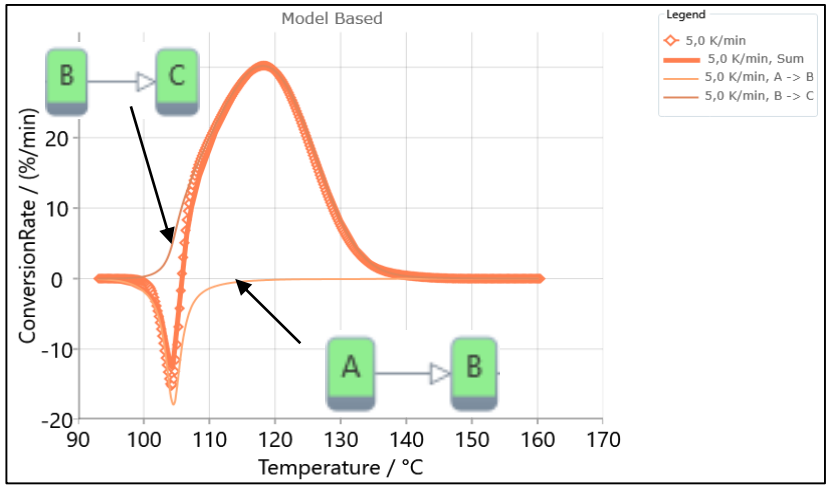


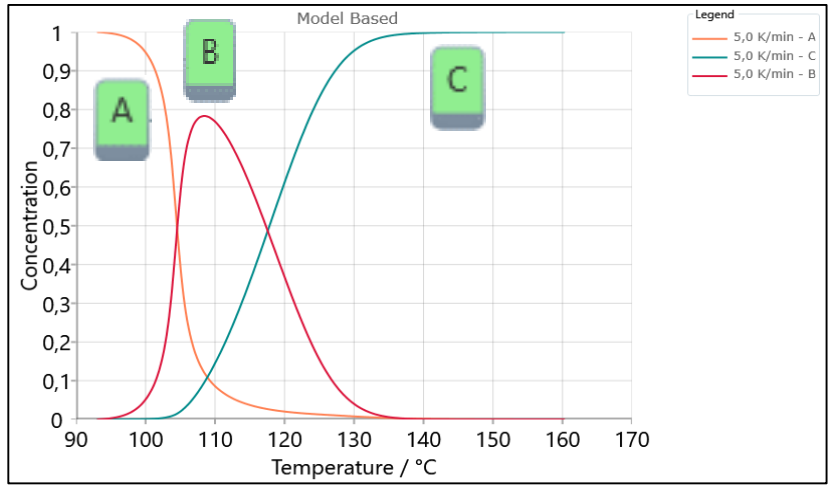
Individual reaction steps



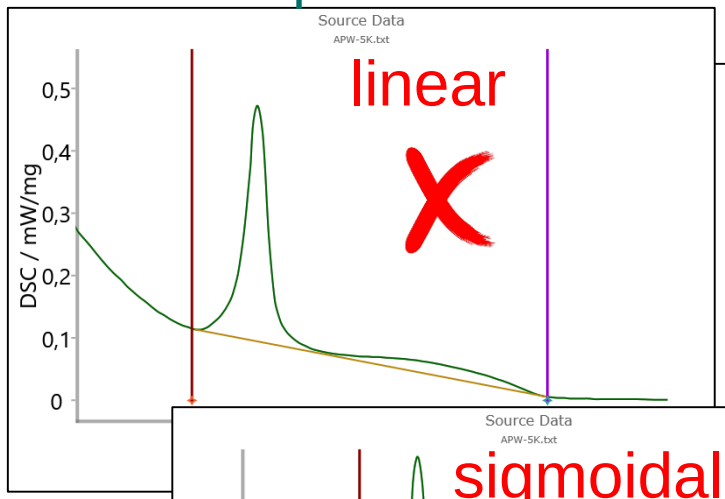
Concentration of reactants

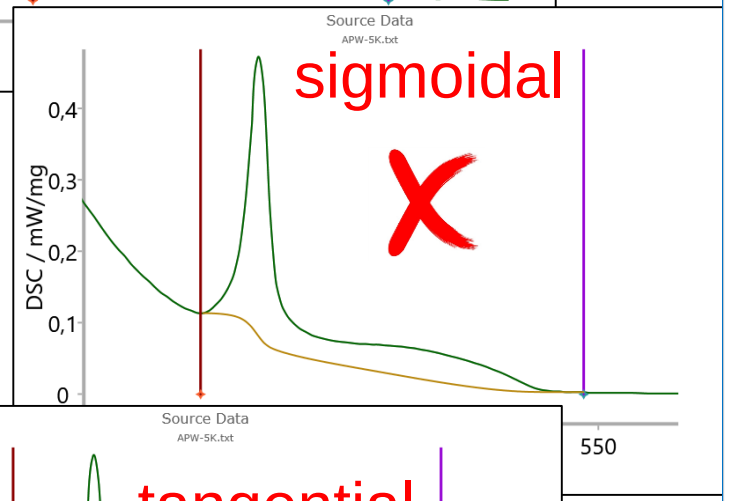


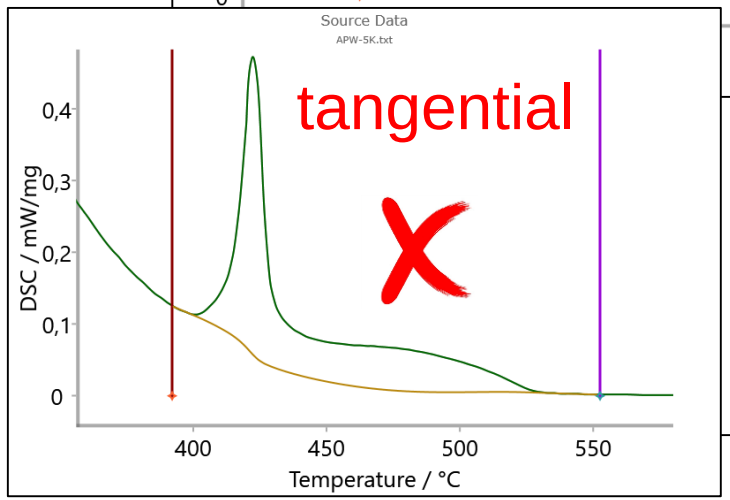


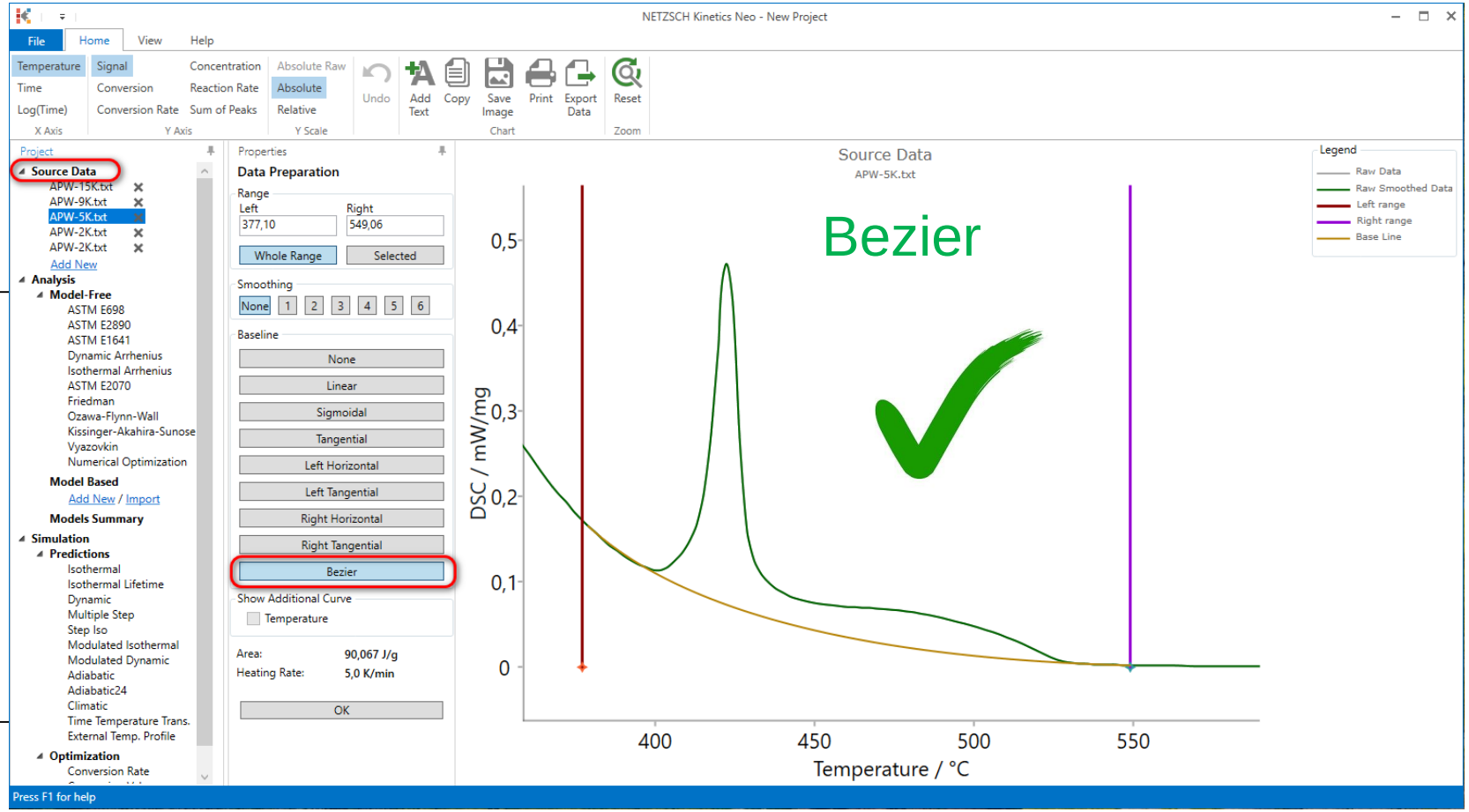


3.6 Unique: Bezier baseline for DSC with background process





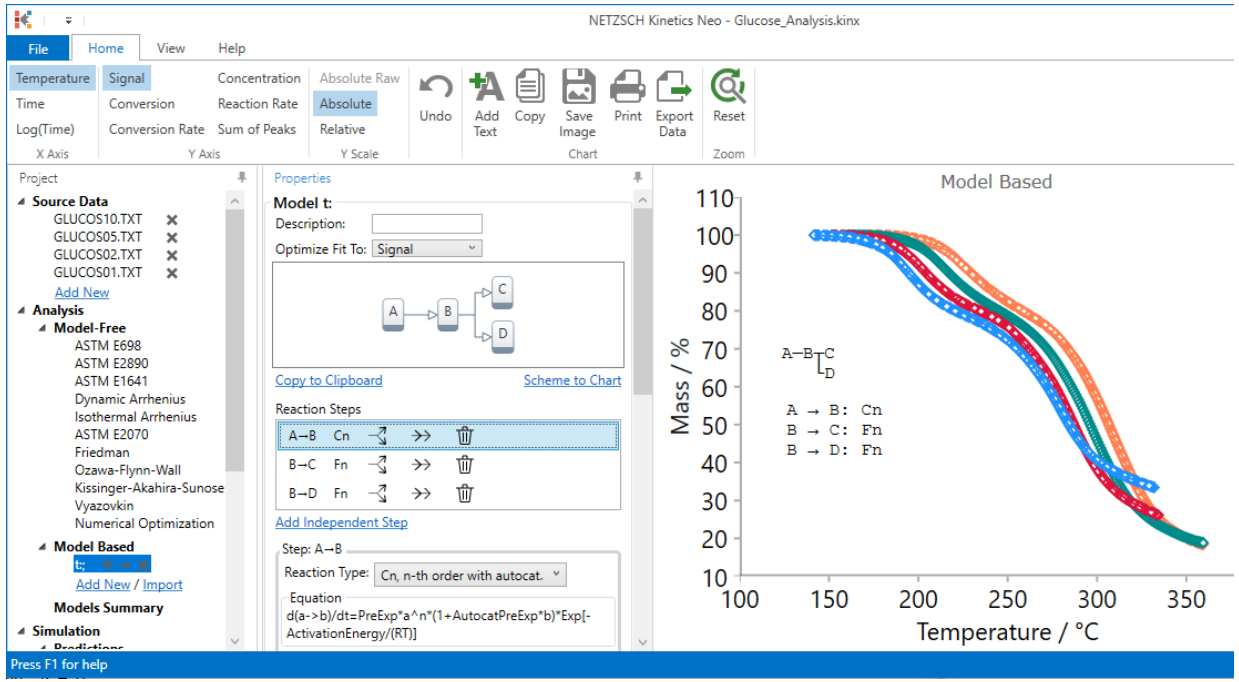


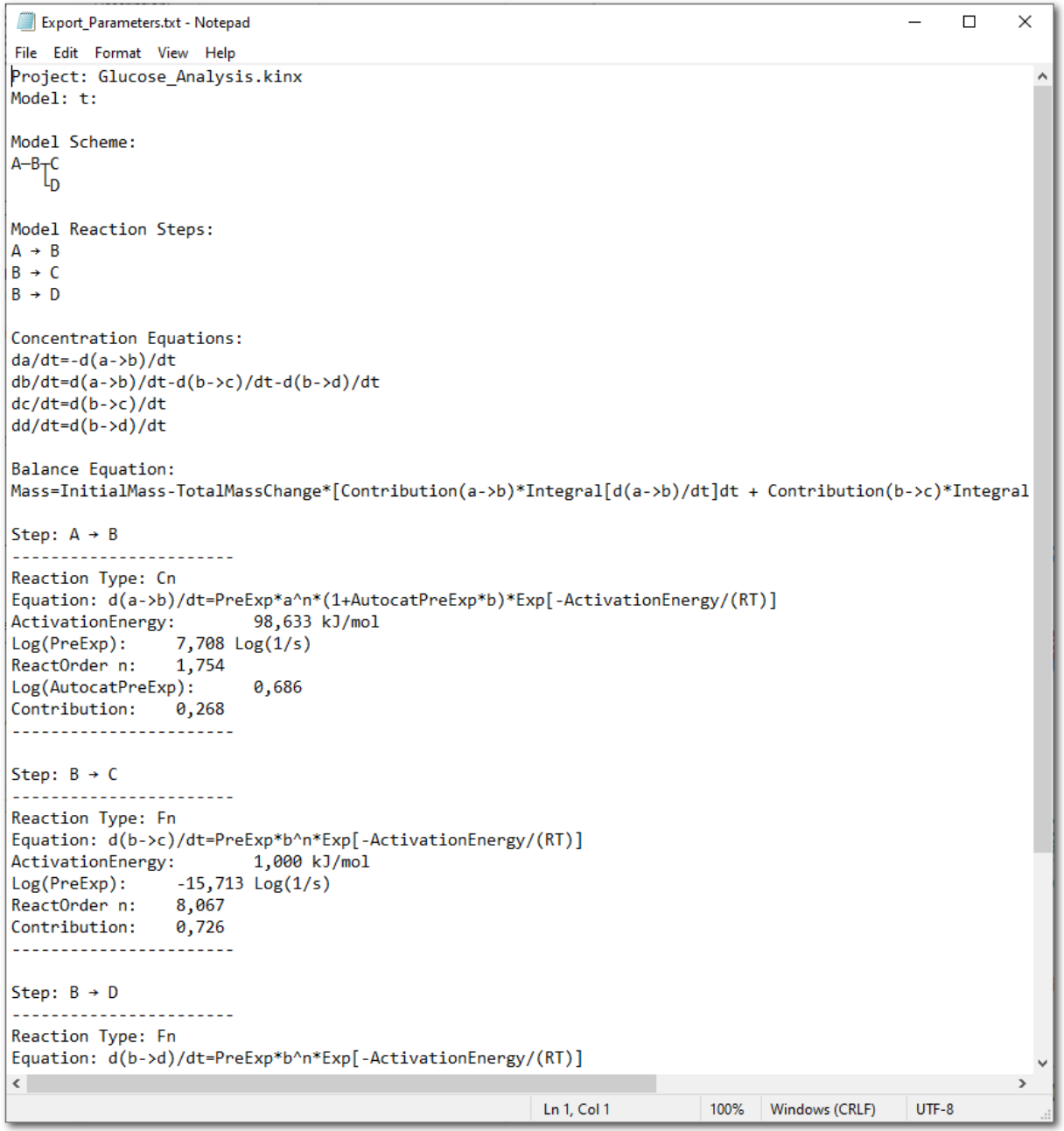


Usage:

- if there is some independent background process (e.g.evaporation) which is not important
- baseline is still instable (e. g. begin of the segment)

3.6 Unique: Export equations





These equations easy in FEM (Finite Element Method) software to simulate

- Temperature distributions
- Concentration distributions

for the volume with any complex geometry

NETZSCH Kinetics Neo Web Site including User Guides

https://kinetics.netzsch.com

Trial Version 30 days

NETZSCH

Learn - Kinetics Neo

https://kinetics.netzsch.com/en/learn/

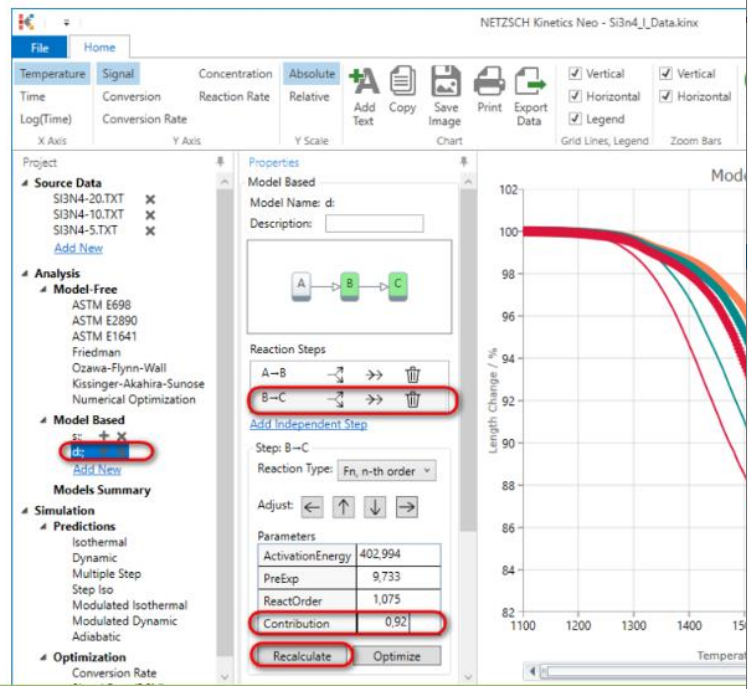
How To: Create a Three

https://kinetics.netzsch.com/en/learn/how-to-dil-3-steps-sintering-of-si3n4/

NETZSCH What Is New Features Learn F.A.Q. Applicat

10. Select the second step and set its contribution to 0.92.

In "Step B -> C" region click "Recalculate" button.



How To: Create TTT Diagram for

https://kinetics.netzsch.com/en/learn/how-to-ttt-diagram-dsc-diffusion-control/

NETZSCH Proven Excellence.

What Is New Features Kinetics as a Service Learn F.A.Q. Applications Support and Service Docs

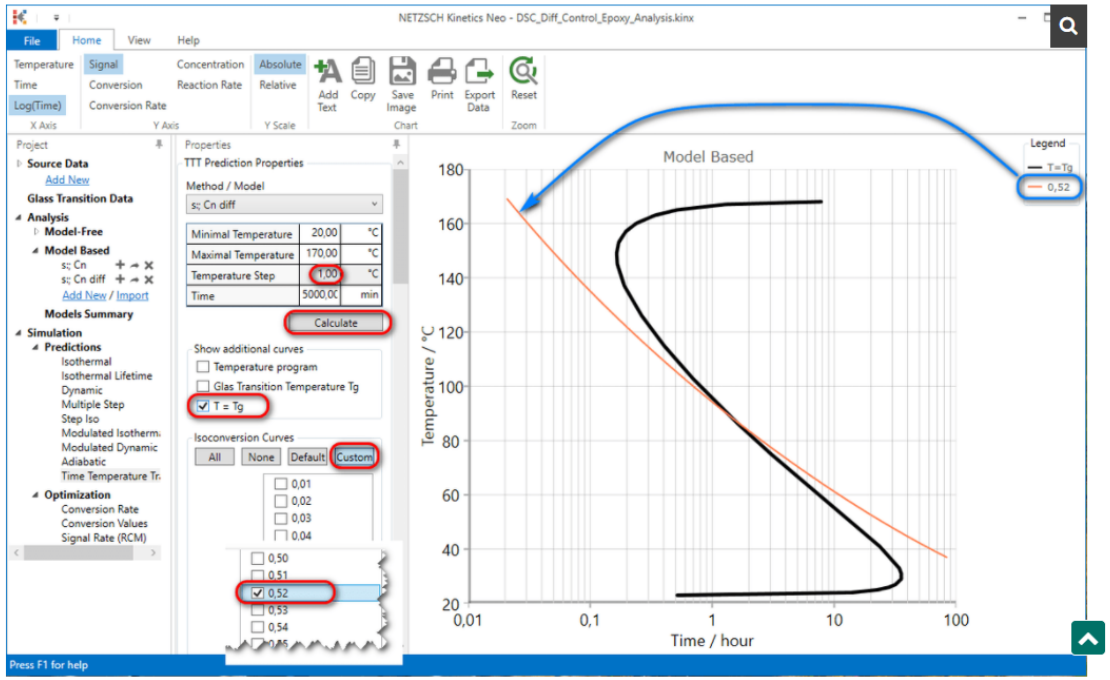
Gelation Curve

12. If the conversion for gelation point is known then gelation curve can be shown. Let us show gelation curve for known conversion value 52%.

Write 1°C for temperature step and turn *Off* **Glass transition Temperature Tg**.

Press *Calculate*.

For *Isoconversion Lines* click *None*, then *Custom* and select one value **0.52**.



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KINETICS NEO is used to analyze kinetics of temperature dependent chemical processes.

Analysis

- one mathematical kinetic description for several measurements
- different approaches: model free (11 methods) and model based (unlimited number of models)
- model based: individual reaction steps, concentrations, kinetic triplet for each step, reaction mechanism
- standard reaction types (n-th order, Autocatalysis, diffusion, Avrami nucleation)
- unique reaction types (Kamal-Sourour, diffusion control, Nakamura nucleation, Hoffman-Lauritzen theory)
- Standard data types like TG or DSC
- Unique data types (Dilatometry, Rheometry, DEA)

Predictions and optimizations

- optimization of industrial chemical processes like debinding, curing, sintering
- standard predictions (isothermal, heating, multi-step, user-defined, TD24, climatic for 100 weather stations)
- unique predictions of individual peaks, concentrations, Tg, TTT diagram, temperature presets like fire presets)
- prediction of viscosity or ion viscosity for new temperature profile
- Optimization of temperature profile for constant or predefined conversion rate

NETZSCH
Proven Excellence.

Thank you for your attention.
Any questions?

webinar_ngb@netzsch.com

https://kinetics.netzsch.com