NETZSCH

Proven Excellence.



Kinetics Neo

Kinetic Analysis Software for Thermal Measurements of Chemical Reactions.
Model-Free and Model-Based Methods

Analyzing & Testing

KINETICS NEO

Substances with well-defined properties can be converted into other substances with different properties by the chemical reactions of a set of reactants. Reactions can run their course within a fraction of a second, as with explosions, or can take thousands or even million of years, as with the formation of minerals. Kinetics, also called reaction kinetics or chemical kinetics, investigates the rates of chemical processes and allows for the determination of reaction rates.

Applications

- Prediction of degree of cure including determination of the curing time during material changes. The simulation accounts for autocatalytic reactions, reactions with diffusion control and changing of the glass transition temperature during the curing process.
  → Automotive and aerospace industry, paints, epoxy coatings, composites, adhesives, etc.
- Viscosity changes during the coating process? → Paints, coatings, adhesives
- Reaction mechanism for complex processes, including information about each reaction step and all its parameters from activation energy and reaction order to the number of reaction steps and their contribution to the total processes.
- Crystallization of polymers during fast cooling → Injection molding
- Optimization of debinding processes to achieve highest quality in shortest time.
  → Sintering during powder metallurgy processes
  → Production of ceramics, sintering behavior
- How long can a pharmaceutical be stored until it loses its activity?
  → Pharmaceutical research and industry
- How long can epoxy coatings or polymer insulations withstand exposure to gases, liquids or electrical lines at a certain temperature or under real climatic conditions present at a selected location on Earth?
  → Packaging industry
- How long can a high-energy material or hazardous substance be safely stored?
  → Chemical and military industry
  → Thermal runaway
- What is the temperature for an adiabatic process with maximum temperature rate in 24 hours (TD24)? →Estimations of thermal risks and hazards

Data Type

TGA, DSC, DTA, DIL, DEA

FOR ANY REACTING MATERIAL…

Kinetics Neo

can analyze any process for which the rate depends on temperature

NETZSCH *Kinetics Neo* software is used to analyze kinetics of temperature-dependent chemical processes. The result of such analysis is a kinetics model or method correctly describing experimental data under different temperature conditions. Use of the method/model allows for predictions of a chemical system's behavior under user-defined temperature conditions. Alternatively, such models can be used for process optimization.

The software can analyze different types of thermal curves that depict the changes in a given material property measured during a process. Potential data sources include studies using thermogravimetry, dilatometry, differential scanning calorimetry, Fourier-Transform infrared spectroscopy, mass spectrometry and rheometry, as well as temperature analysis during adiabatic measurements.

The unique model-based kinetic analysis is capable of determining the number of reaction steps, and for each step the following values:

- Enthalpy (exo/endothermal DSC effects) or mass loss (TGA)
- Reaction type
- Activation energy
- Pre-exponential factor
- Order of reaction
- Order of autocatalysis
- Additional kinetic parameters
- Crystallization parameters

All Kinds of Advantages

The primary advantage of *Kinetics Neo* is its ability to analyze both heterogeneous and phase-boundary reactions – and to analyze such reactions with diffusion and nucleation. Furthermore, reactions with partial diffusion control can be studied; for example, processes which change the state of a substance from the glassy to the non-glassy state.

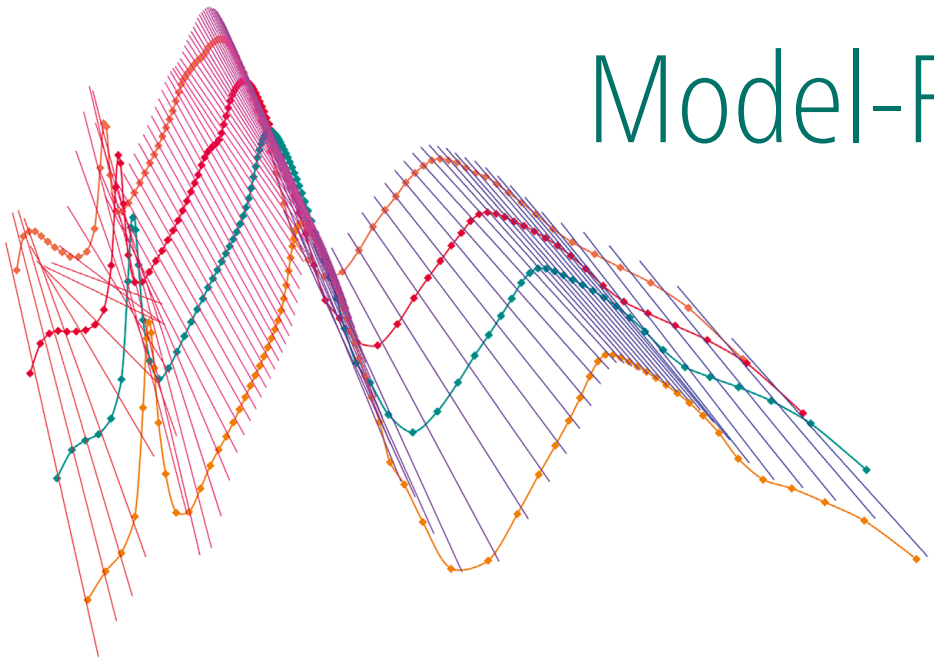
Kinetic Analysis
Model-based or model-free

→

Prediction
of user-defined temperature profile

→

Process Optimization



Model-Free Analysis

Kinetics Neo allows for the use of both model-free and model-based methods.

Starting Points for a Kinetic Analysis

Each kinetic analysis requires a set of analytical measurements carried out under different temperature conditions. These can include dynamic test runs using different heating rates or isothermal measurements monitored at different temperatures. Even a combination of dynamic and isothermal measurements is suitable for kinetic studies.

The Basics of Model-Free Analysis

Model-free analysis allows for the determination of the activation energy of a reaction process without assuming a kinetic model for the process. Also, the reaction type is usually not required to calculate the activation energy.

However, it is not possible to determine the number of reaction steps, their contribution to the total effect or the order in which they occur.

Model-free analysis is based on two assumptions:

1. The reaction can be described by only one kinetic equation for the degree of reaction α :

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

where E(α) is the activation energy depending on the conversion α, and A(α) is the pre-exponential factor.

2. The reaction rate at a constant value of conversion is only a function of temperature.

In addition to having its own specific advantageous features, *Kinetics Neo* is also in accordance with the following standards, common and special methods:

- Analysis
  - Model-Free
    - ASTM E698
    - ASTM E2890
    - ASTM E1641
    - ASTM E2070
    - Friedman
    - Ozawa-Flynn-Wall (OFW)
    - Kissinger-Akahira-Sunose (KAS)
    - Vyazovkin
    - Numeric Optimization

There Is No Assumption of the Reaction Type

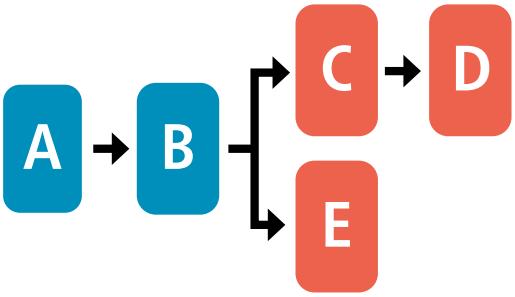
The Model-Free Analysis Methods – Advantages and Disadvantages

The **Friedman** analysis is an isoconversional method whereas the **Ozawa-Flynn-Wall** (OFW) and **Kissinger-Akahira-Sunose** (KAS) analyses are integral isoconversional methods. In all methods, the measurements are analyzed for multiple levels with the same conversion. Friedman requires at least two measurements. In addition to two dynamic measurements, OFW and KAS require positive heating rates.

The **Numerical Optimization** uses digital simulation in determining the activation energy and pre-exponential factor to achieve the best agreement between simulated and experimental curves. At least two measurements are required.

Methods Included in *Kinetics Neo*		Advantage	Disadvantage
Conversion-dependent methods	Friedman	▪ For multiple-step reactions without parallel reaction steps ▪ Evaluation of each reaction point ▪ Suitable for dynamic and isothermal measurements	For parallel and independent reactions, the mean values of E_a are given
	Ozawa-Flynn-Wall (OFW)	▪ For multiple-step reactions without parallel reaction steps ▪ Evaluation of each reaction point	▪ Suitable only for dynamic runs ▪ For parallel and independent reactions, the mean values of E_a are given
	Kissinger-Akahira-Sunose (KAS)	▪ For multiple-step reactions without parallel reaction steps ▪ Evaluation of each reaction point	▪ Suitable only for dynamic runs ▪ For parallel and independent reactions, the mean values of E_a are given
	Vyazovkin non-isothermal	▪ For multiple-step reactions without parallel reaction steps ▪ Evaluation of each reaction point	▪ Suitable only for dynamic runs ▪ For parallel and independent reactions, the mean values of E_a are given
	Numerical Optimization	▪ For multiple-step reactions without parallel reaction steps ▪ Evaluation of each reaction point ▪ Suitable for dynamic and isothermal measurements	For parallel and independent reactions, the mean values of E_a are given
	ASTM E2070	Evaluation of each reaction point	Suitable for isothermal runs only
Methods based on a single conversion	ASTM E698 ASTM E1641 ASTM E2890		▪ Only for one-step reactions; for complex reactions, the points are not on a straight line ▪ Only for dynamic measurements ▪ Only one point is evaluated; all other information is not used

The difference between Ozawa-Flynn-Wall and Kissinger-Akahira-Sunose are in the calculation formula and results. The same is true for the Friedman analysis method and Numerical Optimization.



Model-Based Kinetics – Eliminates All the Disadvantages of Model-Free Analysis Methods

Model-Based Kinetics for Comprehensive Analysis of Chemical Reactions

The extraordinary model-based analysis was developed by NETZSCH. It uses powerful cutting-edge mathematical calculations to create the best kinetic model; the different kinetic models can then also be compared statistically. Therefore, this approach has none of the disadvantages which can be observed when using model-free methods.

The Unique Model-Based Analysis

The Model-Based Kinetic Analysis Is Based on Three Assumptions

1. The reaction consists of several elementary reaction steps, and the reaction rate of each step can be described by a kinetic equation of its own for the given step, depending on the concentration of the initial reactant e_j, the concentration of product p_j, the pre-exponential factor A_j and the activation energy E_j, specific only for this step with number j, as follows:

$$\text{Reaction Rate}_j = A_j \cdot f_j(e_j,p_j) \cdot \exp\left(\frac{-E_j}{RT}\right)$$

   Each step has its own reaction type described by the function $f_j(e_j,p_j)$.

   Some examples of these functions include a second-order reaction which has $f = e^2$, a Prout–Thompkins reaction with acceleration which has $f = e^m p^n$ and a reaction with a one-dimensional diffusion which has $f = 0.5/p$. The number of kinetic equations is equal to the number of reaction steps; the concentration for each reactant increases for the reaction steps where this reactant is a product, and decreases for the reaction steps where this reactant is a starting substance.

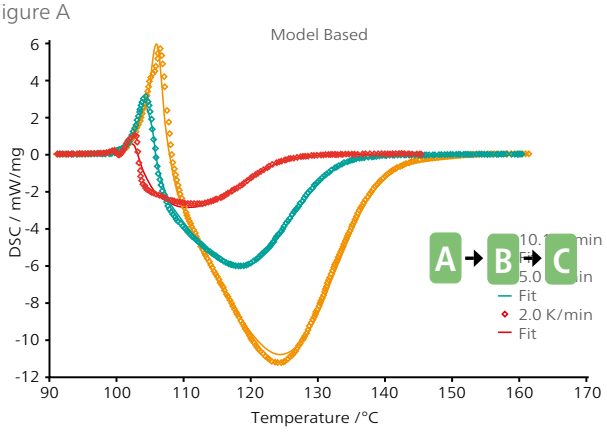
2. All kinetic parameters including the activation energy, pre-exponential factor, order of reaction, and reaction type are assumed to be constant during the reaction progress for every individual reaction step.

3. The total thermoanalytical signal is the sum of the signals of the individual reaction steps. The signal of each step is calculated as the reaction rate multiplied by the total effect of the given step; e.g., total enthalpy change or total mass loss.

   Kinetic parameters are determined by the software to obtain the best fit either for signal (default) or for conversion curves.

Kinetic Model with Consecutive Reaction Steps of Different Directions

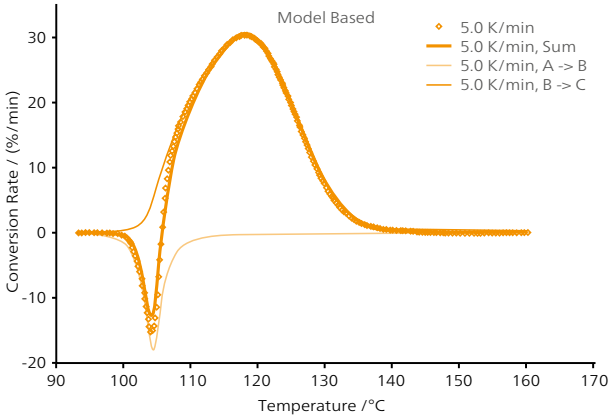
Figure A



Processes with different peak directions or with parallel or highly overlapping steps can be analyzed only by model-based methods. Model-free methods such as Friedman or Ozawa-Flynn-Wall can not be applied for these processes.

The decomposition of AIBN (aso-bis-isobutilonitril) contains two DSC peaks of different directions: the first one is endothermal and the second one exothermal. The model-based method is used here to create a two-step model with two different consecutive steps (Figure A).

Figure B



The kinetic model of several steps can be presented as the sum of the individual peaks, where each peak has a meaning of the individual reaction step. The reaction steps must not be independent for such presentation (Figure B).

The multi-step model contains the individual reactants with changing concentrations. First, the concentration of the intermediate products increases because of initial steps, and then decreases when final products are produced (Figure C).

Time Constant Correction

The heavy DSC crucibles (e.g. high-pressure and medium-pressure) have long time constants and influence the shape of the DSC curve. The DSC signal must be corrected to remove this influence (Fgure D: corrected curve (green) and measurement curve (grey) using high-pressure crucible (27µl)).

Figure C

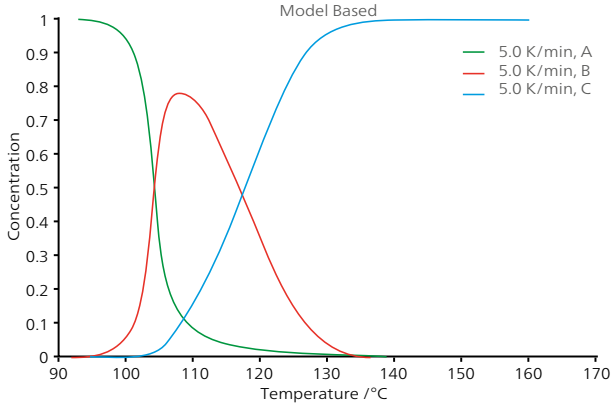
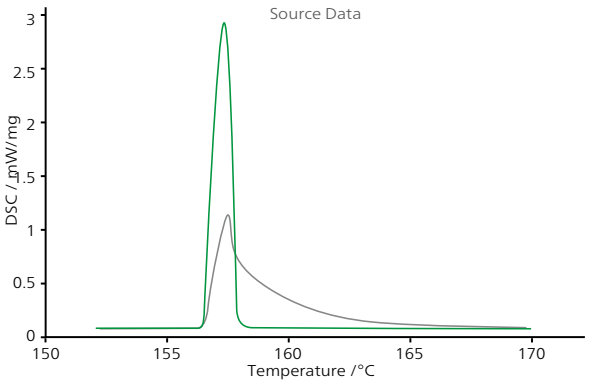
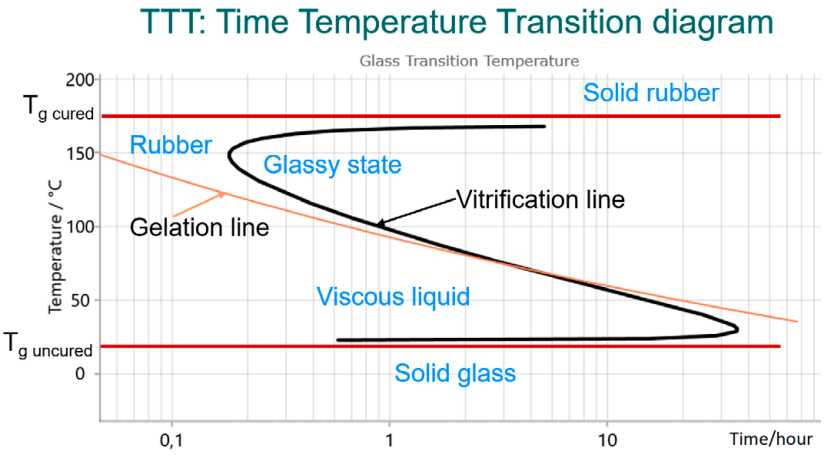


Figure D





Kinetics Neo Includes a Variety of Reaction Types

Code	Function in *Kinetics Neo*	Type of Reaction
F1	$f = e$	Reaction of 1st order
F2	$f = e^2$	Reaction of 2nd order
Fn	$f = e^n$	Reaction of nth order
R2	$f = 2e^{1/2}$	Two-dimensional phase boundary
R3	$f = 3e^{2/3}$	Three-dimensional phase boundary
D1	$f = 0.5/p$	One-dimensional diffusion
D2	$f = -1/\ln(e)$	Two-dimensional diffusion
D3	$f = 1.5e^{2/3} /(1 - e^{1/3})$	Three-dimensional diffusion – Jander's type
D4	$f = 1.5/(e^{-1/3} - 1)$	Three-dimensional diffusion – Ginstling-Brounstein
B1	$f = e \cdot p$	Prout-Tompkins equation
Bna	$f = e^n \cdot p^a$	Expanded Prout-Tompkins equation
SB	$f = e^n \cdot p^m \cdot [-\ln(e)]^q$	Extended Sestak-Berggren equation
C1	$f = e \cdot (1 + \text{AutocatOrder} \cdot p)$	Reaction of 1st order with autocatalysis by product
Cn	$f = e^n \cdot (1 + \text{AutocatOrder} \cdot p)$	Reaction of nth order with autocatalysis by product
Cmn	$f = e^n \cdot (1 + \text{AutocatOrder} \cdot p^m)$	Reaction of nth order with autocatalysis of mth order by product
Kamal-Sourour	Two parallel reactions with the same reactant and the same product. One is the reaction of the nth order, the second is the autocatalytic reaction with its own activation energy	
A2	$f = 2e \cdot [-\ln(e)]^{1/2}$	Two-dimensional nucleation according to Avrami
A3	$f = 3e \cdot [-\ln(e)]^{2/3}$	Three-dimensional nucleation according to Avrami
An	$f = n \cdot e \cdot [-\ln(e)]^{(n-1)/n}$	n-dimensional nucleation according to Avrami-Erofeev
Nk	$n \cdot e \cdot [-\ln(e)]^{(n-1)/n} HL(T)$	Nakamura crystallization with Hoffman-Lauritzen temperature dependence HL(T) and Avrami nucleation An
SbC	$e^n \cdot p^m \cdot [-\ln(e)]^q HL(T)$	Sbirrazzuoli crystallization with Hoffman-Lauritzen temperature dependence HL(T) and extended Sestak-Berggren nucleation SB

Each reaction step j is of a certain reaction type which is mathematically included via the function $f_j(e_j,p_j)$. *Kinetics Neo* includes all listed types of reaction.

Predictions

Trial-and-error is finally a thing of the past!

Based on the created kinetic model (model-free or model-based), the software simulates the signal, conversion rate and conversion for user-defined temperature programs. This allows for the prediction of sample properties for temperature conditions which differ from the conditions originally used during the measurement(s).

Careful kinetic analysis of the experimental data is recommended prior to the calculation of predictions.

Long-term prediction of material aging, including prediction under real climatic conditions or prediction of time-to-failure at a given temperature, can be carried out using the Arrhenius approach in cases where no complete measurement is available. The initial data used are the failure temperature during heating (e.g., OIT or specimen fracture during DMA tests) and the experimental time-to-failure under isothermal conditions.

The prediction for external temperature profiles helps find the reaction behavior for temperatures recorded during industrial processes or find the decomposition during firing by using pre-defined temperature presets.

Predictions

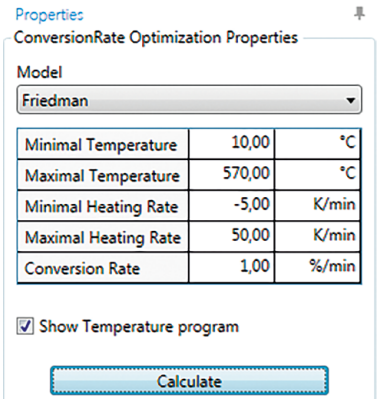
- Isothermal
- Isothermal lifetime
- Dynamic
- Multiple step
- Step iso
- Modulated isothermal
- Modulated dynamic
- Adiabatic
- Adiabatic24
- Climatic
- Time-Temperature-Transition (TTT)
- External temperature profile

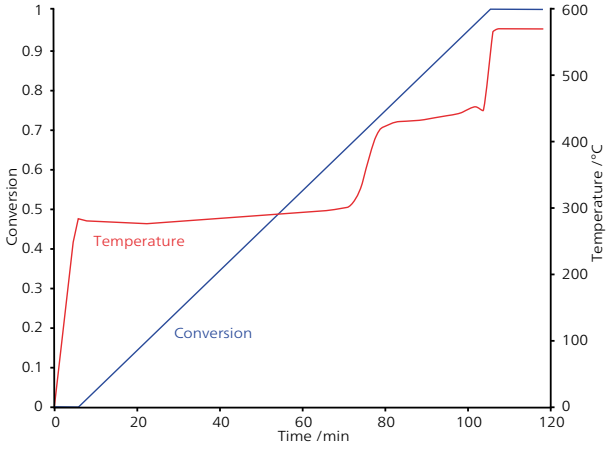
Optimization

- Conversion rate
- Signal rate (RCM for thermogravimetry and RCS for dilatometry)

Process Optimization

This feature allows for the simulation of data once the experimental data is described by model-free or model-based kinetics. The temperature profile can be calculated and optimized taking into account defined boundary conditions; e.g., constant or user-defined conversion rate, constant signal rate, temperature range and range of heating rates. The results depend on the chosen model-free or model-based method and its parameters. Careful kinetic analysis of the experimental data is required prior to calculating the optimization (see column at right).





Optimization of the conversion rate at 1 %/min



What Makes *Kinetics Neo* So Valuable ...

- Completely rewritten from scratch, this innovative software is based on the latest technologies.
- The improved user interface is fast and easy to operate.
- All model-free and model-based methods are included. The results from all of these methods can be statistically compared with one another.
- The powerful new numerical model-free method ensures fast determination of the best model-free solution.
- Predictions and optimizations can be achieved by means of both model-free and model-based methods.
- A visual kinetic model can be created quickly and easily using the model-based method.
- Unlimited number of kinetic models.
- The kinetic model can contain any number of individual reaction steps in any combination. Reaction steps can be easily added, removed or changed by the user.
- The position of individual reaction steps can be visually adjusted at any time.
- An individual step or the entire kinetic model can be optimized with just a click of the mouse.
- The software can present the curve of its reaction rate as the sum of the separated peak curves of individual reaction steps
- The software provides the formal concentration of each reactant and reaction rate for each reaction step as a function of time or temperature.
- Crystallization processes for isothermal and cooling conditions can be analyzed and predicted.

MODEL-BASED

PREDICTIONS

OPTIMIZATION

VISUAL ADJUSTMENT

ANY NUMBER OF REACTION STEPS

ISOTHERMAL AND DYNAMIC CRYSTALLIZATION

NEW MODELS

COMBINATION OF REACTION STEPS

FAST AND EASY-TO-USE INTERFACE

TTT DIAGRAM

IN ACCORDANCE WITH STARDARDS

MODEL-FREE

Simulation for Reliable Predictions and Process Optimization

Analyzing the Curing Behavior of an Epoxy-Based Adhesive

- **What is the minimum temperature needed for a specified cure over a given duration of time?**
- **What is the degree of curing for a given temperature program?**

If the glass transition occurs during the cross-linking of a thermoset, the reaction is divided into two areas which are dominated by different mechanisms: The part above the glass transition depends on the chemical reaction and can be described by the Arrhenius relation. In the vicinity of the glass transition, the diffusion-controlled mechanisms dominate the reaction behavior. Therefore, the reaction rate around the glass transition is influenced by both processes, requiring the kinetic model to be extended by the special diffusion control algorithms to take into account the change in material behavior.

Figure A shows the DSC data (points) of a curing process at seven different heating rates and the simulation based on a model with diffusion control in solid lines. This kinetic model is used to calculate the prediction of the reaction rate at different temperature conditions.

Figure B exhibits the experimental glass transition temperatures at different degrees of curing. The solid line is the fit according to the Di Benedetto equation.

Figure C depicts curing behavior for many isothermal conditions. The curing reaction slows down at higher conversion values due to diffusion control, e.g., 90% conversion is achieved at 110°C after 52 min, at 120°C after 26 min, and at 140°C after 8.7 min.

Figure D shows Time-Temperature-Transition diagram (TTT diagram) for a longer time period.

Figure A

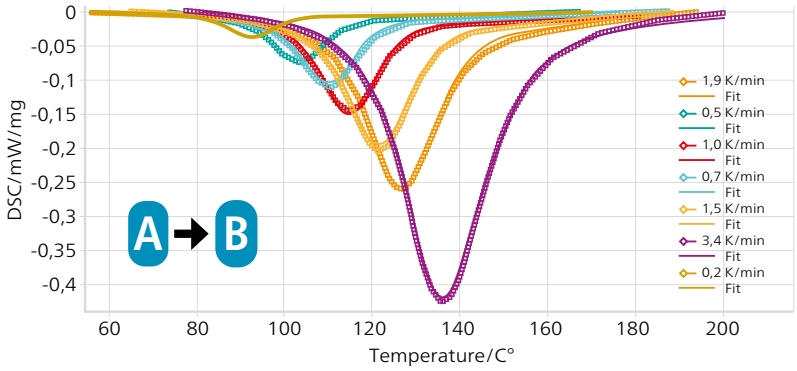


Figure B

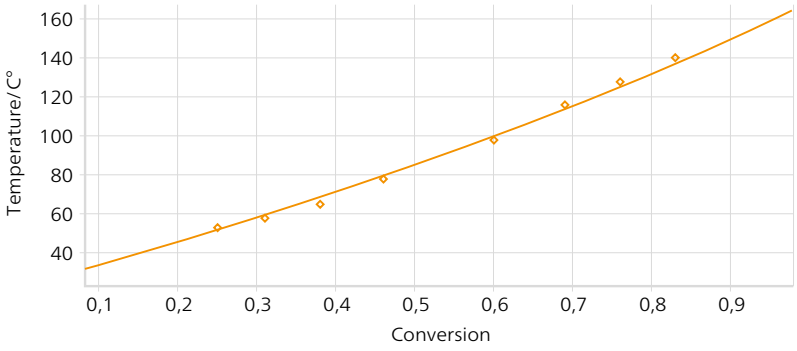


Figure C

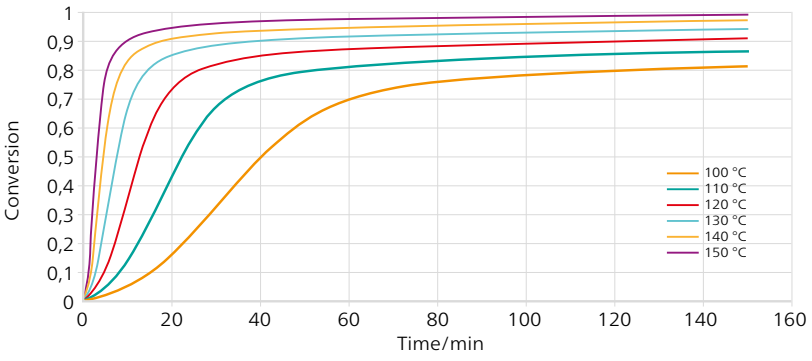
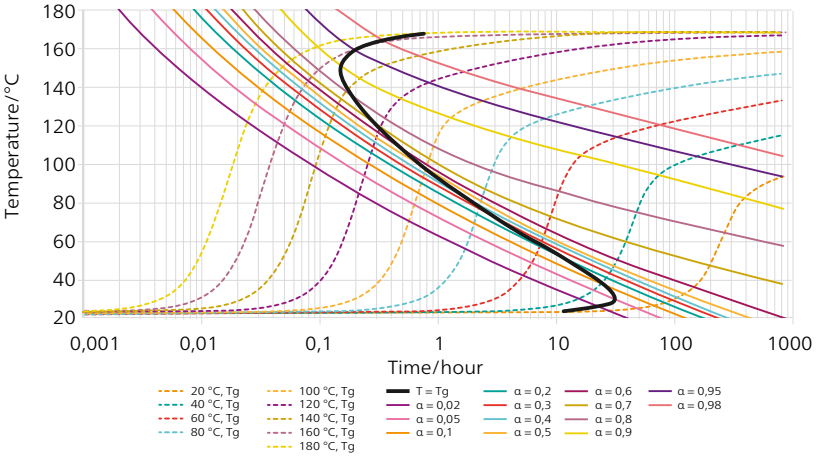


Figure D



Polymer Crystallization Kinetics During Cooling or Isothermal Conditions

Selective Laser Sintering (SLS): PA12

It is very important to know the crystallization rate, what fraction of the polymer becomes crystalline, and what fraction is in the glassy state at low temperatures.

Figure A presents the experimental data (points) and simulation (solid lines) according to the Sestak-Berggren kinetic model for isothermal crystallization of PA12.

Figure B presents the crystallization simulation of polyamide 12 during SLS on the top layer of powder fusion bed for the measured temperature curve (lower curve). The low degree of crystallization (upper curve) after one laser cycle shows that the complete crystallization takes place during several powder layers.

Injection Molding: PET

In the production of PET bottles, firstly the PET preform is manufactured by an injection molding process, and then PET preforms are expanded with compressed air to the bottle shape.

Figure C shows the experiment and model according to Nakamura for non-isothermal crystallization during cooling. It also describes the large decrease in the peak area for fast cooling.

Figure D exhibits the prediction of crystallization at different isothermal temperatures beween 110°C and 150°C after fast cooling during the injection molding process. With decreasing isothermal temperature, crystallinity decreases and the amorphous content increases.

Figure A

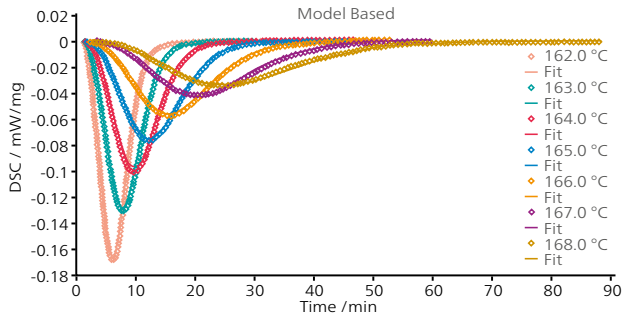


Figure B

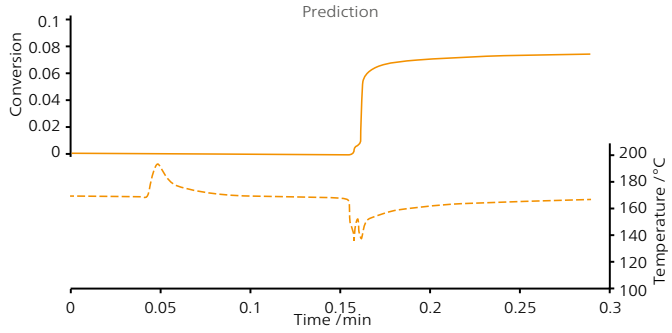


Figure C

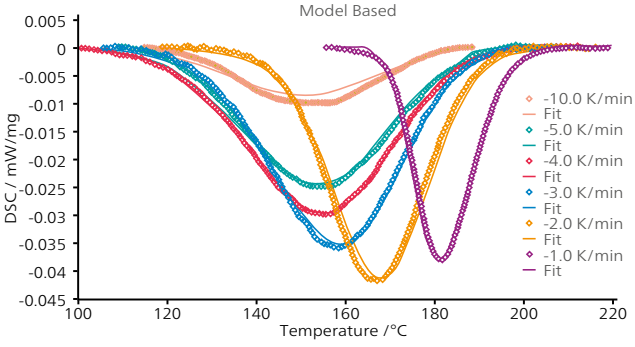
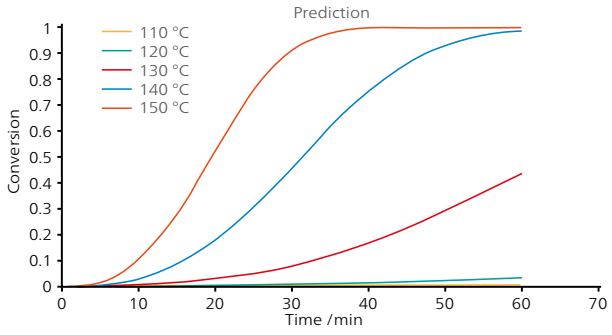


Figure D



Optimization of the Burnout Process of a Polymer Binder for Improved Product Quality

In sinter metallurgy, the added polymeric binder provides improved adhesion to the metal powder. However, if the 1st heating phase is too quick, outgassing of the binder may cause micro-cracking. For the production process, this means finding a good balance between the following two problems:

- **Slow heating results in an increased process time.**
- **Fast heating leads to quality defects due to intensive gas evolution during polymer decomposition.**

Therefore, the optimum temperature profile over all zones of the tunnel kiln has to be determined to ensure a favorable relationship between process duration and product quality.

Figure A shows thermogravimetric measurements carried out at different heating rates. The three-step model used here allows for a high-quality approximation of all measurements. The higher the fit quality, the more confident the predictions.

Figure B shows the optimum temperature profile for the polymer burnout under laboratory conditions. For the best material quality, a constant mass-loss rate of 0.05%/min should be maintained over the entire process.

Figure C depicts the mass-loss prediction in a 5-zone tunnel kiln for a temperature program corresponding to the optimum zone temperatures for the polymer burnout during the production process.

Figure A

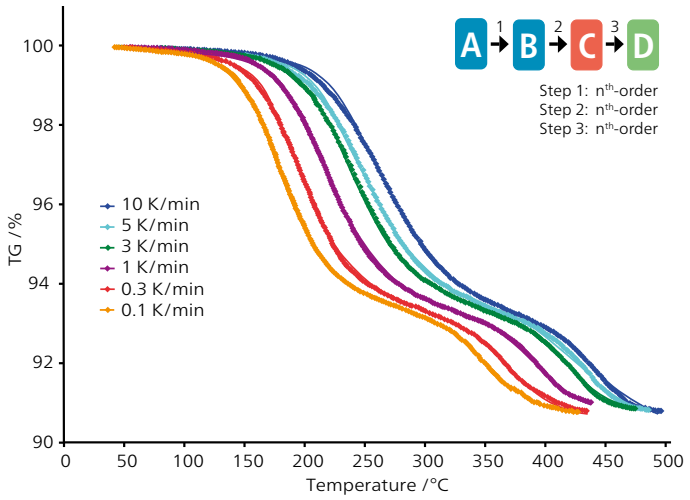


Figure B

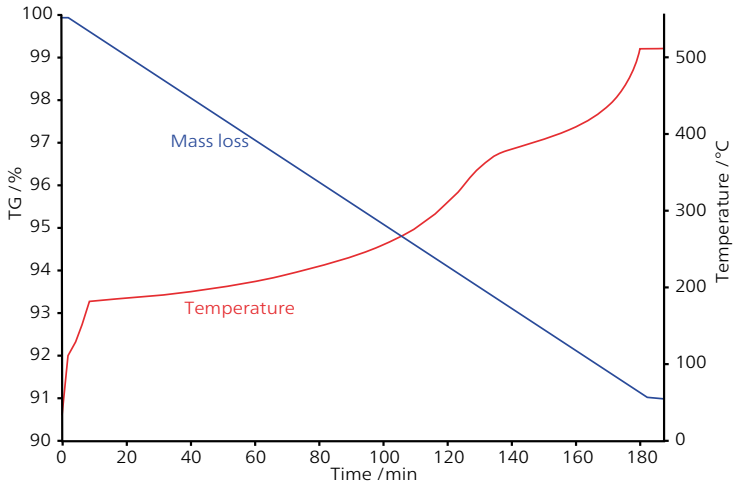
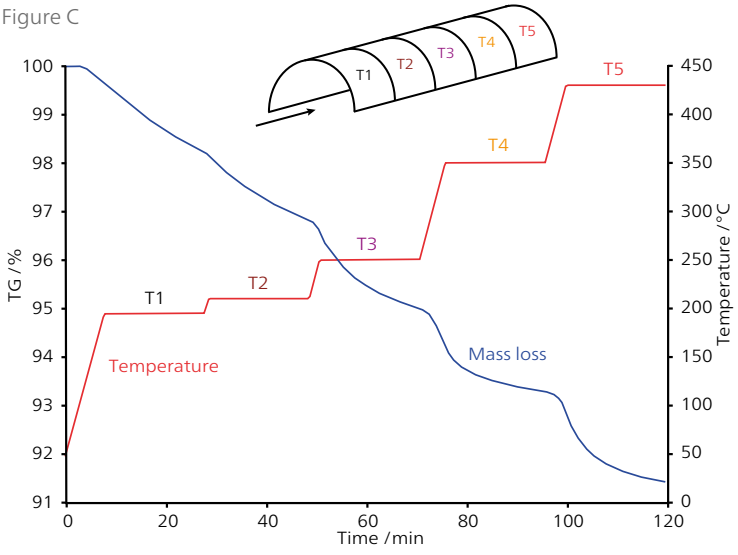


Figure C

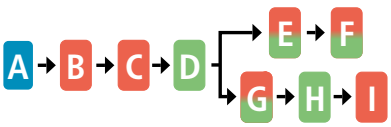


What Exactly Happens During Thermal Decomposition?

Understanding Complex Chemical Reactions – Tracking Decomposition Pathways

The decomposition of ammonium paratungstate tetrahydrate (APT) as studied under an oxidizing atmosphere using four heating rates with the NETZSCH STA simultaneous (TGA-DTA/DSC) thermal analyzer (figure A). In order to better understand the various endo- and exothermal effects of this complex decomposition process, the STA 449 ***F1*** *Jupiter*® system was coupled to the QMS for simultaneous evolved gas analysis (EGA).

From the kinetic analysis of the MS data for water (figure B; measured points and calculated solid lines) and ammonia (figure C; measured points and calculated solid lines), it was possible to determine the decomposition path as a system of consecutive and competing reactions. On the basis of the kinetic model and the quantified MS data according to the known initial amount of N and O in APT, it was possible to determine the entire path, as follows:



Kinetic model of the decomposition of APT·2.9H_2O (blue): partial steps for water (red) and ammonia (green).

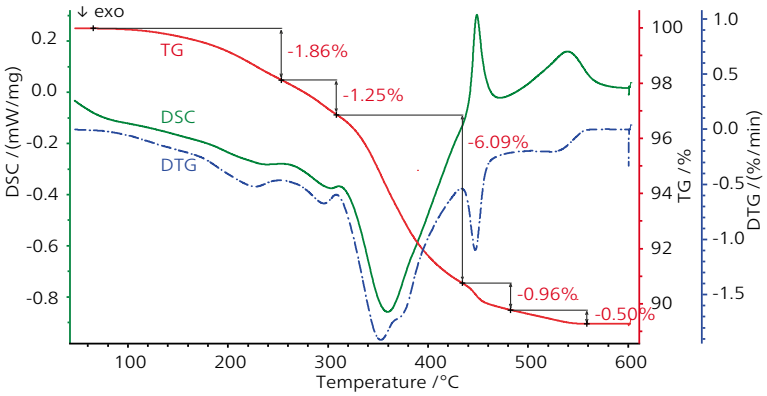


Figure A: STA measurement of the decomposition of APT

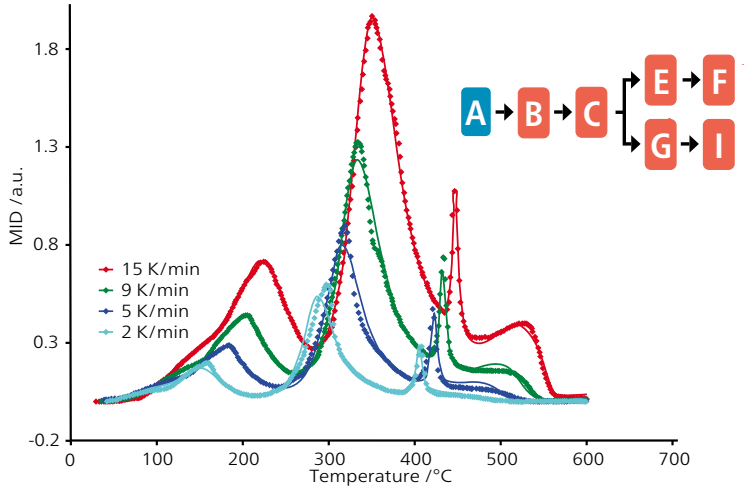


Figure B: Model-Based; MS spectra of the water release at different heating rates

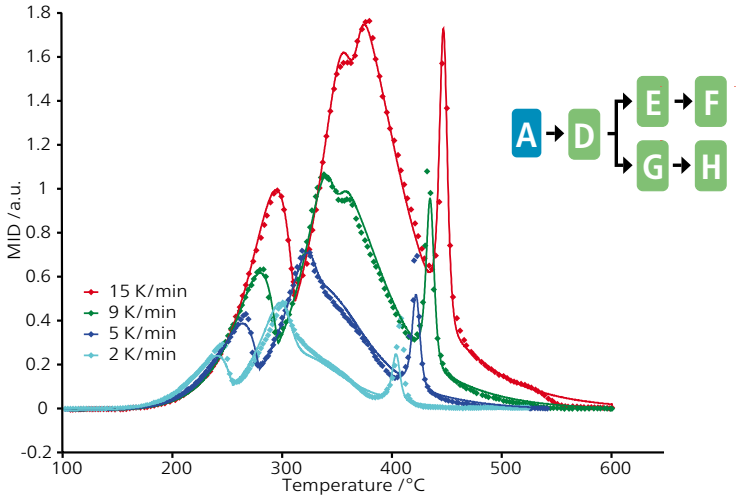


Figure C: Model-Based; MS spectra of the ammonia release at different heating rates

Optimization of Sintering Processes

Tuning the Product Quality of High-Tech Ceramics – Si_3N_4 Green Body

The temperature program during the firing process of a ceramic green body, most of all during the binder burnout and sintering phase, has paramount influence on the later product quality. By modifying the temperature program of a dilatometer measurement, it is possible to optimize the properties of sintering products; e.g., densification and grain size distribution.

Figure A shows the length change (sintering) between 1050°C and 1850°C under the influence of different heating rates. As the heating rate increases, sintering is shifted to higher temperatures. For the kinetic analysis, a 4-step model was employed. Based on this model, a non-linear regression was carried out adjusting the different reaction parameters, such as pre-exponential factors and activation energies (solid lines; measurement data is depicted in points).

It becomes possible to calculate the sintering process for different temperature profiles or for constant shrinkage rates. Figure B depicts the temperature profile for rate controlled sintering (RCS) at a constant length change rate of 0.087%/min.

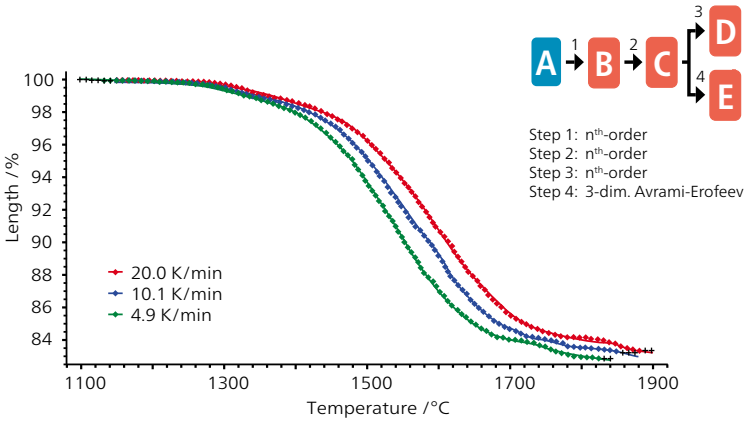


Figure A: Dilatometer measurements on Si_3N_4 powder containing 5 m% of Y_2O_3 and 5 m% of Al_2O_3 as sintering additives. The tests were carried out with the NETZSCH DIL 402 *Expedis*.

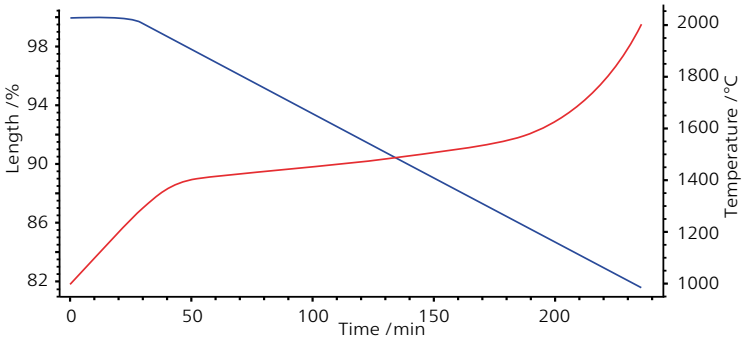


Figure B: Predicted temperature profile for RCS at a constant length change of 0.087%/min

Optimization of the Sintering Process via Kinetic Analysis on the Basis of Dilatometer Measurements

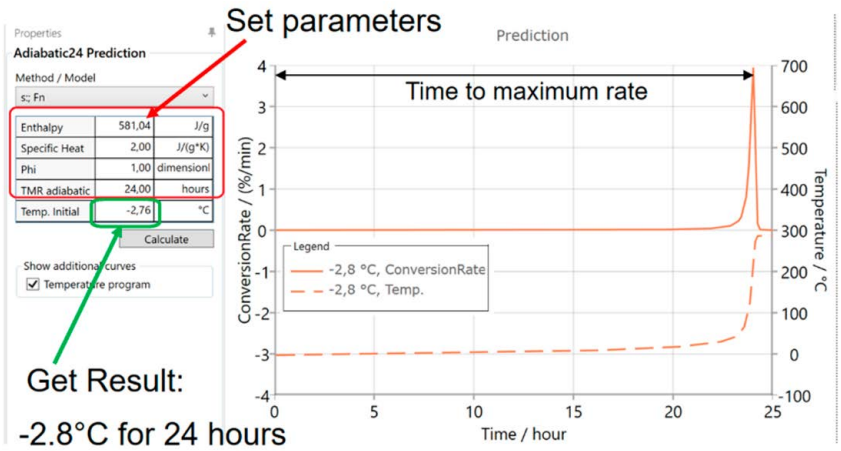
Kinetics Neo finds the temperature program for a given reaction rate or a given rate of final product production.

Special Predictions

Adiabatic24 (TD24) for Estimations of Thermal Risks and Hazards

This feature calculates the initial temperature for an adiabatic process at maximal temperature rate in 24 hours

Figure A: presents the calculated TD24 for at -2.8°C.



Prediction of Viscosity

In this example, kinetic analysis of rheological data (Figure B) during the curing process is used for the prediction of the viscosity for a user-defined temperature program (Figure C).

Figure B

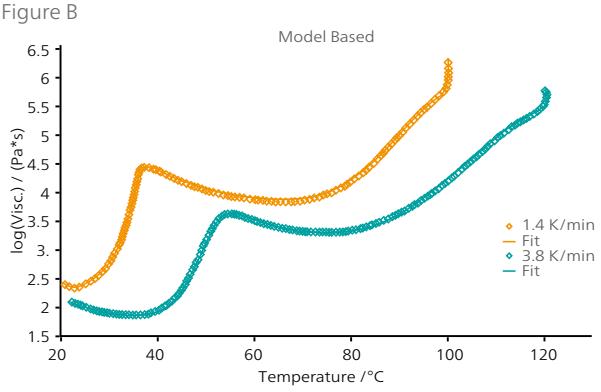
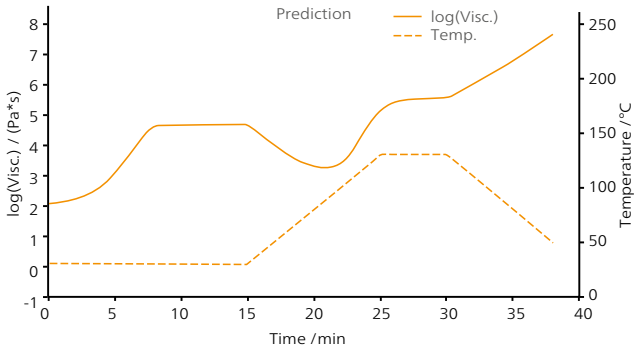


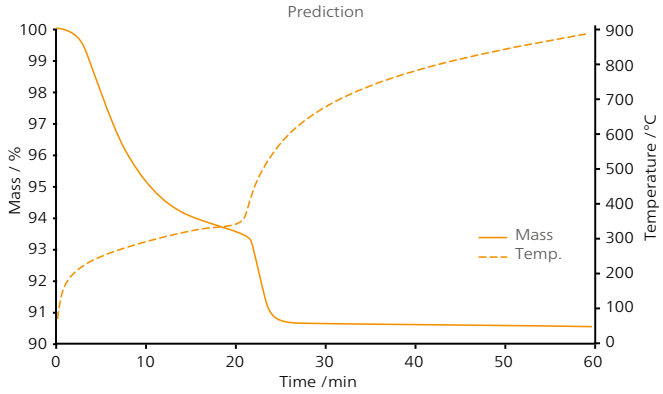
Figure C



Behavior of Non-Flammable Materials Under Firing Temperatures

The composition behavior of non-flammable materials under fire conditions answers the question: How is the degradation behavior of building materials and constructions under fire exposure?

Figure D



Kinetics Neo contains the presets for the fire curves in accordance with the following standards:

- ISO 834-1
- EN 1363-1
- EN 1363-2
- EN 1991-1-2

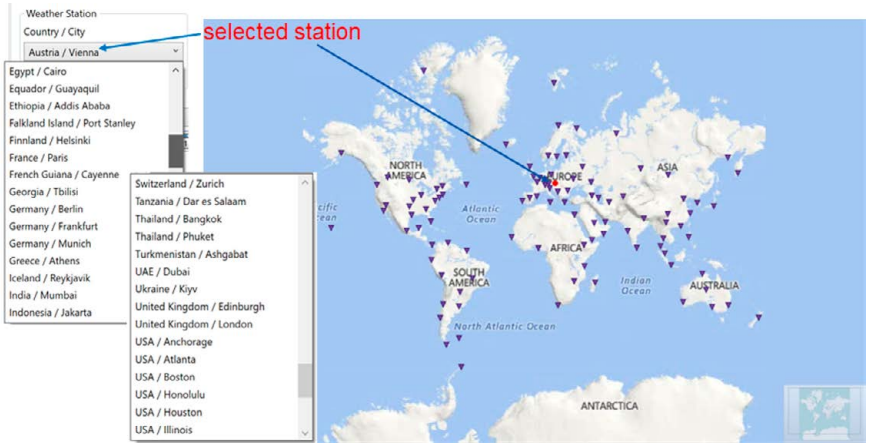
The fire curves:

- Standard time-temperature fire curve
- Hydrocarbon curve
- External fire curve
- Slow heating curve

Predictions Based on Climate Temperature Profile

These predictions in *Kinetics Neo* allow for predictions of a reaction progress for the real atmospheric temperatures. This is possible from any selected point on the Earth, for any selected day of the year, for any duation from months or even years.

The software contains historical data for 1,3,5,10 and 30 years for each of more than 100 weather stations, with minimal and maximum temperature of each day of the year.



These predictions are important for:

- long storage under the climatic temperature conditions
- degradation processes of packaging and coating
- curing of paints or epoxy
- safe storage of high energetic materials

Dehydration of Calcium Hydrogen Phosphate Dihydrate

Kinetic modelling based on TGA measurements (Figure A) are long-term predictions for this process simulated under different climatic temperatures in Paris (Figure B) and Jakarta (Figure C). These predictions were calculated for the time frame of 2 years.

Figure A

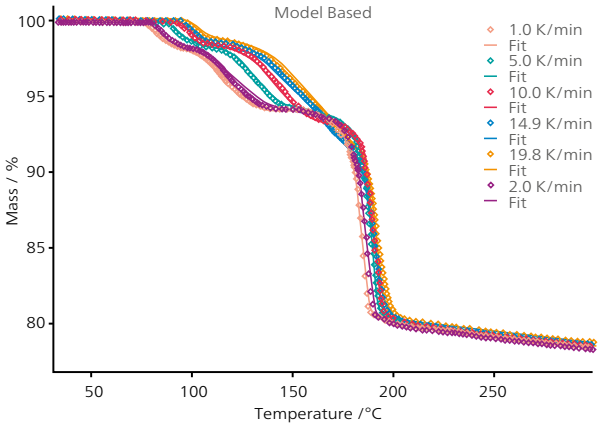


Figure B

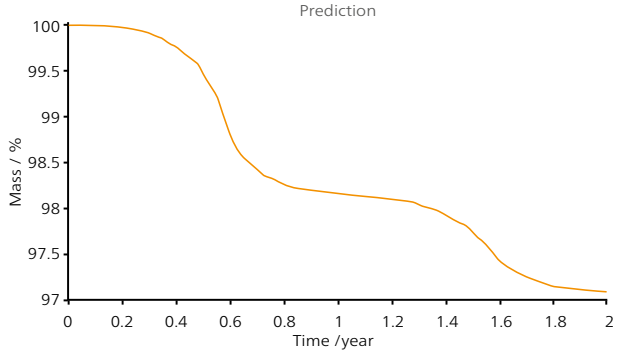
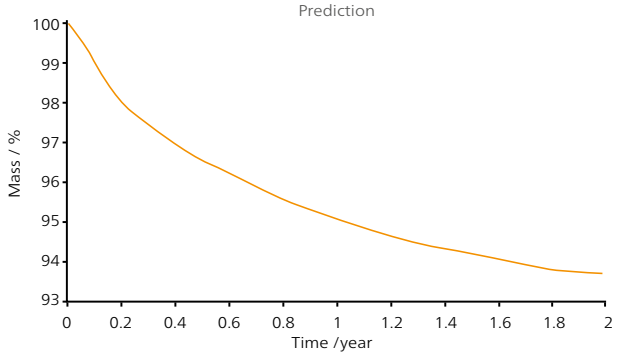
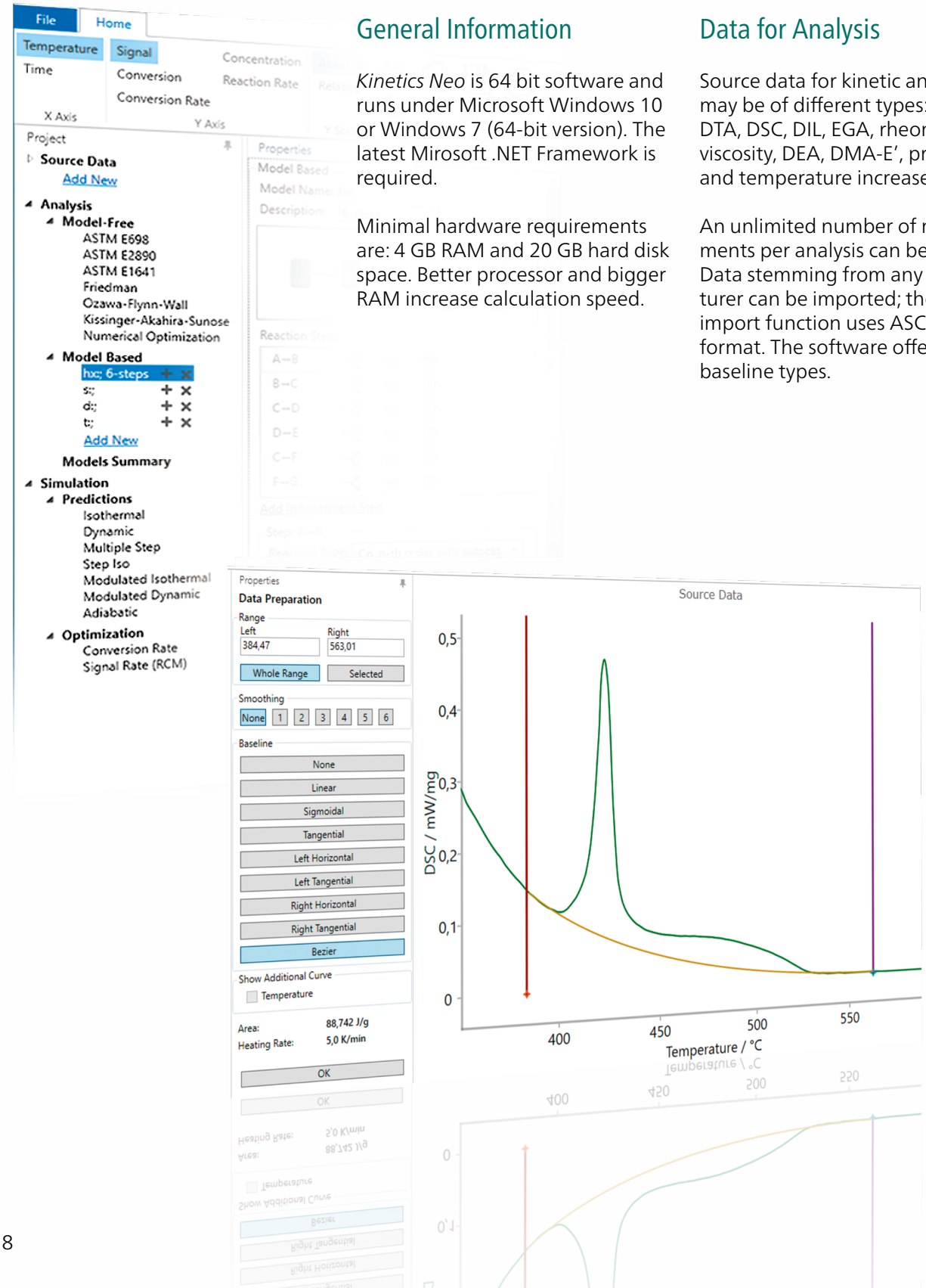


Figure C



SOFTWARE DETAILS



General Information

Kinetics Neo is 64 bit software and runs under Microsoft Windows 10 or Windows 7 (64-bit version). The latest Mirosoft .NET Framework is required.

Minimal hardware requirements are: 4 GB RAM and 20 GB hard disk space. Better processor and bigger RAM increase calculation speed.

Data for Analysis

Source data for kinetic analysis may be of different types: TGA, DTA, DSC, DIL, EGA, rheometry, viscosity, DEA, DMA-E', pressure, and temperature increase.

An unlimited number of measurements per analysis can be used. Data stemming from any manufacturer can be imported; the data import function uses ASCII or CVS format. The software offers various baseline types.

Is the model ready? You're just a click away from predicting and optimizing your process for many different conditions!

Model-Free Methods – Results

- Analysis graph with Y-axis:
  - log (heating rate),
  - log (heating rate/T^2)
  - log dx/dt versus 1000/T
- Plots of activation energy and pre-exponential factor vs. conversion
- Master plot for f(α)
- Conversion fit

Unique Flexible Model Designer

Model-based kinetic analysis offers the possibility of visual design for kinetic models with an unlimited number of steps connecting in any combinations.
The models can be flexibly designed by adding new reactions as independent, consecutive or competitive steps to any place in the model.
A simulated reaction step can be visually moved to the corresponding step on the experimental curve. Then the parameters of this step can be optimized.

Model-Based Methods' Results

Approximately 95% of all chemical reactions are multi-step reactions. This requires a multi-step analytical engine as offered by the *Kinetics Neo* software. The engine uses non-linear regression methods and allows for the optimization of parameters for individual steps or for the complete model. The fit results present the agreement between the experimental and simulated curves for:

- Signal
- Conversion
- Conversion rate
- Concentration of all reactants
- Reaction rates for all steps
- Equations for reaction rate, concentrations, balance equation for signal
- Conversion rate as the sum of separated peak curves for individual reaction steps

Model-Based Methods – Statistical Results

The statistical results incorporate:

- Correlation coefficient
- Sum of the squares of deviations
- Mean residual
- t-value
- F-test for fit quality
- F-test for a number of steps
- Durbin-Watson value
- Durbin-Watson test

Predictions



Predictions can be calculated under various conditions (see also page 8). Depending on the condition, the results can be demonstrated in various ways including:

- Conversion curve as a function of time with temperature as a parameter
- Concentration over time of the formal reactants with temperature as a parameter
- Partial reaction, mass loss and area
- Reaction rate for individual reaction steps
- ... and many more.

Process Optimization

The goal is to develop a suitable temperature program for optimum product quality without trial and error. The results of the optimization can be achieved for:

- A constant rate of output signal like RCM or RCS
- A constant conversion rate

The owner-managed NETZSCH Group is a leading global technology company specializing in mechanical, plant and instrument engineering.

Under the management of Erich NETZSCH B.V. & Co. Holding KG, the company consists of the three business units Analyzing & Testing, Grinding & Dispersing and Pumps & Systems, which are geared towards specific industries and products. A worldwide sales and service network has guaranteed customer proximity and competent service since 1873.

When it comes to Thermal Analysis, Calorimetry (adiabatic & reaction), the determination of Thermophysical Properties, Rheology and Fire Testing, NETZSCH has it covered. Our 60 years of applications experience, broad state-of-the-art product line and comprehensive service offerings ensure that our solutions will not only meet your every requirement but also exceed your every expectation.

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