Technical Datasheet: **Kinetics Neo 2.0**

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At a Glance – Highlights of Kinetics Neo

Purpose	Kinetics Neo is a software for studying chemical kinetics (reaction kinetics). It investigates the reaction rates of chemical processes depending on time and temperature. Kinetics Neo contains 10 model-free methods including numerical methods for the best model-free results. Kinetics Neo features a unique model-based method that allows for analyzing multi-step processes, determines a kinetic model, makes predictions and optimizations based on this model.
Kinetic analysis	The software uses both model-free and model-based methods. The results of these methods can be statistically compared with one another. Model-free methods determine the activation energy and pre-exponential factor as functions of the conversion degree. Model-based methods determine the kinetics model including • Number of reaction steps • Step contribution to the total effect Parameters for each step are: • Reaction type • Activation energy • Reaction order
Predictions	Based on results of the model-free method or on the created kinetic model, the software simulates the reaction rate and conversion for any user-defined temperature program. This allows for prediction of the sample properties for temperature conditions which differ from the originally measured conditions.
Optimization	Kinetics Neo can optimize the temperature program in order to achieve the desired system behavior, either for a constant conversion rate or for a given rate of production of the final product. Optimization can be achieved by means of both model-free and model-based methods.

System Requirements, General Data of the Software

Operating systems	Microsoft® Windows 7, Windows 8, Windows 8.1, Windows 10 32- or 64-bit
Application language	English
Integrated help system	Context-sensitive, browser-style HTML help interface
Minimal hardware requirements	Desktop PC, laptop or tablet PC; Intel® Core i5 processor, 8 GB RAM, hard disk space 20 GB, display 1440 x 1050
Software delivery	Internet download. CD version is available as a paid option.

Data for Analysis

Data type for kinetic analysis	• DSC • DSC with Diffusion Control • DTA • TGA • DIL • DEA • ARC temperature • Viscosity • Rheometry
Number of measurement data	Unlimited
Import	• Data import can be done from plain text ASCII file, CSV file. Data should contain either three columns (time, temperature, signal) or two colulmns (time and signal or temperature and signal) and the value of the heating rate. • Data can be imported from the projects of Thermokinetics3.
Baseline types	- Linear - Horizontal area proportional - Tangential area proportional - Horizontal left starting - Horizontal right starting - Tangential left starting - Tangential right starting - Zero - Bezier - Linear expansion (DIL) - Heating/cooling (DIL) - Left horizontal (DEA isothermal) - Left tangential (DEA dynamic) - Right tangential (DEA dynamic) - Tangential (DEA dynamic) - Left horizontal (viscosity) - Left tangential (visosity) - Left horizontal (ARC temp. HWS) - Left horizontal (ARC temp) - Tangential ARC (temp)

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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 • 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 and contribution 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 16 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 Models for glass transition function for diffusion control • Di Benedetto model • Splines
Kinetic results	The software determins the kinetics model including • Number of reaction steps • Step contribution to the total effect The standard parameters for each step are • Reaction type • Activation energy • Reaction order Additional parameters for some reaction types • Order of autocatalysis • Dimension of nucleation or diffusion
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

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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	Predicitons for several heating rates
Multi-step prediction	Prediction for a user-defined sequence of dynamic and isotherml 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, respesenting 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.
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 The simulated values can be presented: • Curves as a function of time • Curves as a function of temperature • Table with simulated values, time and temperautre

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 The simulated values can be presented: • Curves as a function of time • Curves as a function of temperature • Table with simulated values, time and temperautre

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File Operations, Graphics and Export	
Graphical presentation of data and results	Presentation of the data in graphic format having X-axes as temperature, time, or logarithm of time. Y-axes in absolute scale or relative scale from minimal to maximal value for each curve with data of • 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
Graphical options	• Add vertical and/or horizontal grid • Add legend • Add any number of arbitrary text blocks to the graphics
Export	For all data, analysis results, predictions and optimizations as well as for all model-free plots, the following operations are enabled: • ASCII export of results including measured data and simulated curves as well as activation energies and pre-exponential factors for model-free analysis • Copy graphics to clipboard • Saves graphics as a picture to PNG format For model-based analysis: • Equations for reaction rate for each individual reaction step in the kinetic model • Equations for concentration of each reactant • Balance equation for total signal like DSC/TGA/DIL, etc. • Copy the image of model to clipboard • Export model into file • Import model from file

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