Technical Data Sheet: *Termica Neo* 1.0

Highlight of *Termica Neo* – Simulation of Thermal Behavior of Large Sample Volumes	
Purpose	*Termica Neo* is a software for the simulation of the thermal behavior and thermal safety for chemical reactions and crystallization in solids or liquids in volumes with sizes from centimeters to meters. Main applications are materials with high thermal potential, as well as reactions of curing, cross-linking, sintering and polymer crystallization.
Software	64-bit software
Simulation	Based on the model-free or model-based kinetics approaches, the software simulates the dependence on time at each point of the reactors for the following parameters: ■ Temperature ■ Conversion ■ Conversion rate ■ Glass transition temperature, T_g, for curing reactions with diffusion control ■ Concentrations of individual reactants in multi-step reactions The simulation uses the environment/surrounding performed for any user-defined temperatur program.
Optimization	Based on the model-free or model-based kinetic approaches, the software can find the surrounding temperature for the reaction behavior defined by the customer like Self-Accelerating Decomposition Temperature (SADT).

System Requirements	
Prerequisites	Kinectis Neo version 2.5 or later
Operating systems	x64 versions Microsoft Windows 11 or Windows 10
Application language	English
Integrated help system	Context-sensitive, online help web site
Minimal hardware	Intel® Core i5 processor 11 Generation (Core i5 11400) or later, 16GB RAM, DirectX 11 compatible graphics, display 1440x1050
Recommended hardware	Intel® Core i7 processor 11 generation or later, 24 GB RAM, graphics nVidia 1080 GTX or better, display 1920x1200

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Data for Simulation

Reactant	Kinetic parameters and equations are based on a previous kinetic evaluation and are loaded directly from the Kinetics Neo project (.KNX2, support by Kinetics Neo Version 2.5 or later); they include: **Possible data type:** ■ DSC ■ DSC with diffusion control ■ DTA ■ TGA ■ DIL ■ DEA ■ ARC Temperature ■ Viscosity **Analyiss type:** ■ Model-free ■ Model-based with unlimited number of individual reaction steps and their combinations including parallel, competing and follow-up reactions **Heat source:** ■ Reaction/crystallization ethalpy **Material library with temperature-dependent physical properties for reactants** ■ Specific heat capacity ■ Density ■ Thermal conductivity **Material phase:** ■ Solid or viscous liquid with negligible convection ■ Liquid with stirring (no temperature gradient) Number of reactants for simulation in one project: unlimited
Container	**Geometry:** ■ Slab infinite ■ Cylinder infinite ■ Cylinder ■ Sphere **Material library with temperature-dependent physical properties for the container:** ■ Specific heat capacity ■ Density ■ Thermal conductivity **Surfaces:** ■ Each surface contains own container material, container thickness surround material and surrounding temperature
Surrounding	**Material library with temperature-dependent physical properties for surrounding:** ■ Heat transfer coefficient for surficial heat exchange ■ Emissivity cofficient **Material library contains special surroundings:** ■ Adiabatic (not heat loss) ■ Infinite (infinite heat loss where the container temperature is equal to the surrounding temperature) **Types of surrounding temperature profiles:** ■ Isothermal ■ Dynamic at constant heating ■ Multiple steps ■ Step iso ■ Modulated isothermal ■ Modulated dynamic ■ External temperature profiles

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Simulations	
Results	■ Temperature T ■ Conversion α ■ Conversion rate dα/dt ■ Glass transition temperature T_g for curing reactions with diffusion control ■ Concentraions of individual reactants in multi-step reactions
Optimization	■ SADT: Self-accelerating decomposition temperature

Visualization Charts and Graphs	
Graphical presentation of data and results	■ Two-dimensional: curves for T, α, dα/dt, concentrations, T_g as a function of time at any user-defined point of the volume. Could be presented as the set of curves having different spatial coordinates ■ Two-dimensional chart (for one-dimensional geometry): curves for T, α, dα/dt, concentrations, T_g as a function of spatial coordinate at any user-defined time point. Could be presented as the set of curves having different time values. ■ Three-dimensional: surface for T, α, dα/dt, concentrations, T_g as a function of time and one selected special coordinate, where other facial coordinated are set to constant value. ■ Heatmap for T, α, dα/dt, concentrations, T_g as a function of time and one selected spatial coordinate, where other spatial coordinated are set to constant value. ■ Cross-section: Three-dimensional surfaces for T, α, dα/dt, concentrations, T_g as a function of two spatial coordinates at the selected time point. ■ Cross-section: Heatmap for T, α, dα/dt, concentrations, T_g as a function of two spatial coordinates at the selected time point.
Export	For all data, simulation and optimizations of the following operations are enabled: ■ ASCII export of results ■ Copy graphic to clipboard
Graphical options	■ Selection of the visual theme for user interface ■ 2D chart o show/hide • legend • grid • zoom bars o select • legend, font • axis font • axis thickness ■ 3D chart o rotate 3D suface o show/hide • color surface • contour lines • wireframe o select • gradient/levels color palette • orthogonal/perspective projection mode • Llghting and opacity effects ■ Heatmap chart o show/hide • color surface • contour lines • grid lines • datapoints for polar plot o select gradient/levels color palette

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