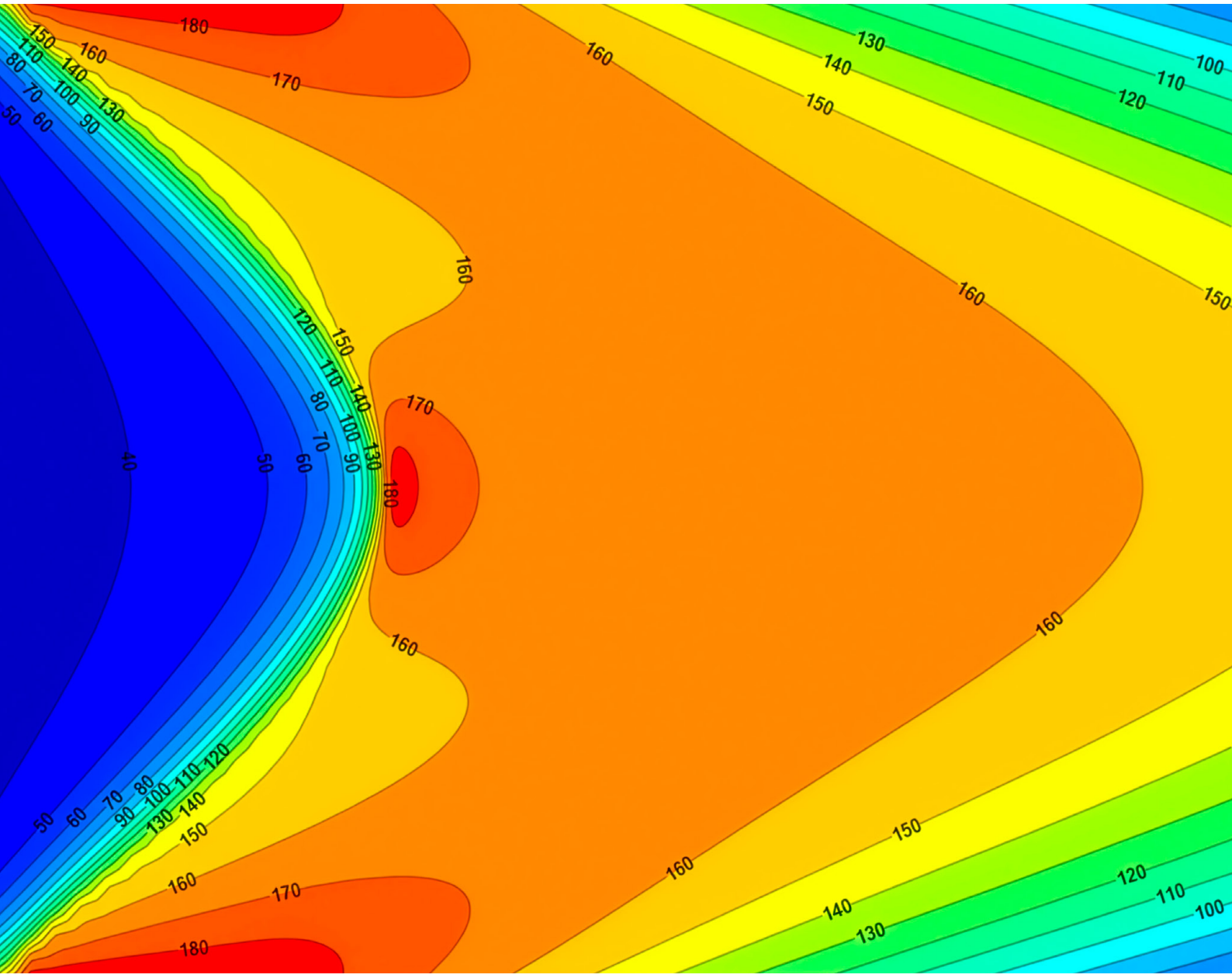
NETZSCH

Proven Excellence.



TERMICA NEO

Software for the Thermal Simulation of Chemical Reactions on an Industrial Scale

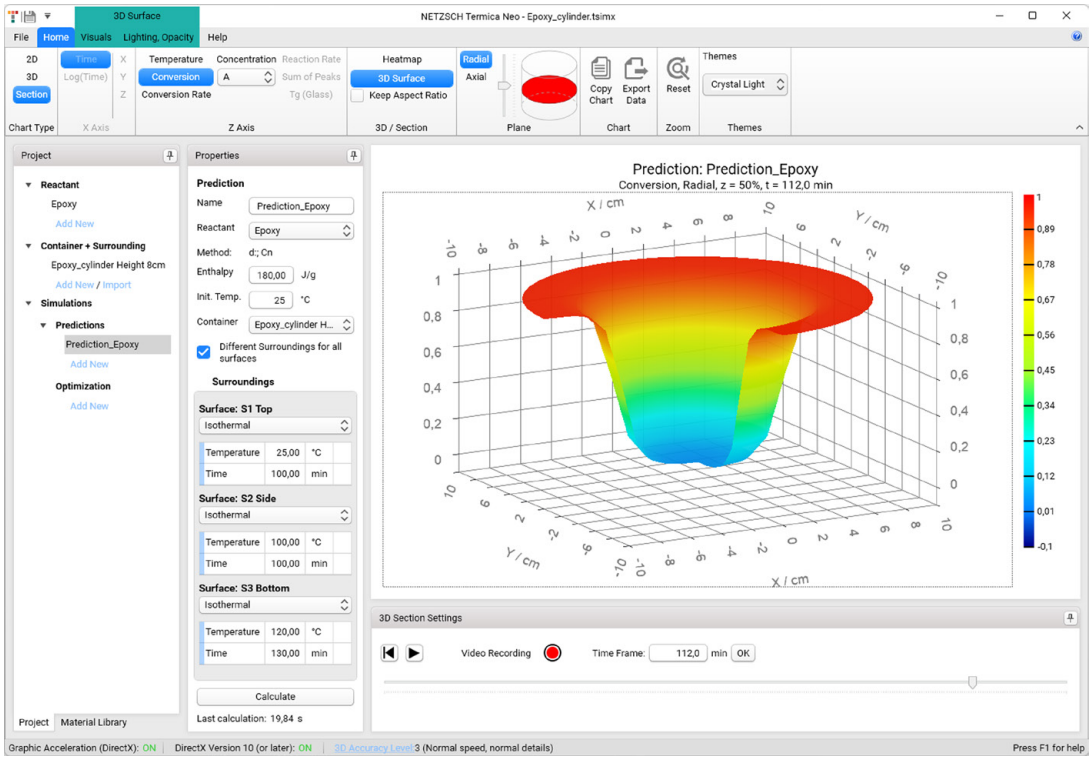
Analyzing & Testing

TERMICA NEO

Termica Neo is a software program designed for the simulation of thermal behavior and thermal safety in chemical reactions and crystallization in solids or liquids. It operates in volumes with characteristic size ranging from centimeters to meters. Primary applications of Termica Neo involve materials characterized by elevated thermal potential, in conjunction with reactions such as curing, cross-linking, sintering, decomposition, and polymer crystallization.

The Strenghts of Termica Neo

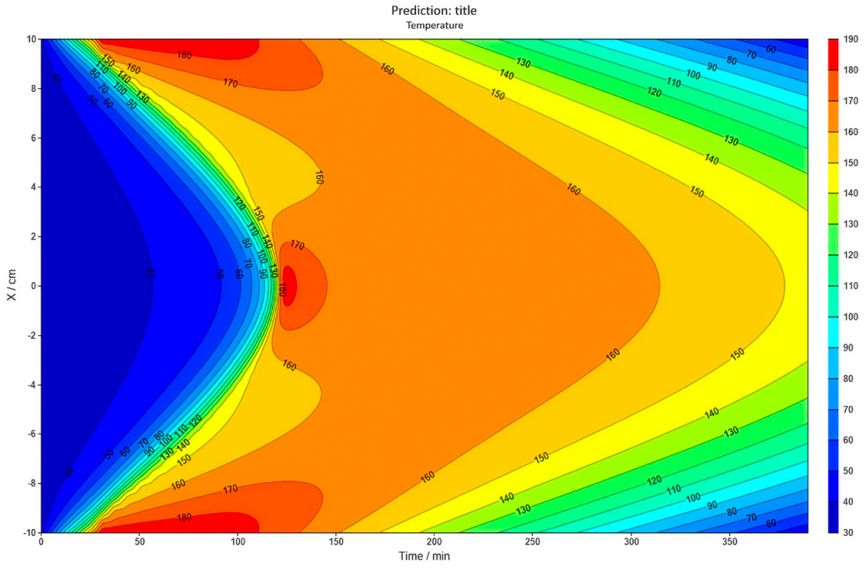
- Simulate the behavior of your material at any point inside the container.
- Determine the location and timing of the maximum temperature or maximum conversion rate of the reactant inside the container.
- Calculate temperature, conversion, and concentrations of the reactant at a given time and position within the container.
- Predict the degree of curing, decomposition, and crystallization.
- Determine thermal safety conditions for production and storage such as SADT.



Impression of the software Termica Neo: intuitive handling, clear structure

What Makes Termica Neo So Valuable

- Fast and easy-to-handle user interface similar to Kinetics Neo.
- The kinetic models are taken directly from the Kinetics Neo project (results of any method including both model-based and model-free).
- Calculation of the following properties at each point of volume as a function of time:
  - Temperature
  - Conversion
  - Conversion rate
  - Concentrations
  - Glass transition temperature
  - Calculation of the Self-Accelerating Decomposition Temperature (SADT) using various materials, containers and surroundings
- Simulation of reactions for a reactor with container, including adiabatic conditions (predictions)



Prediction of the time-dependent temperature distribution within a cylinder

From Data Input to Final Results

Reactant

Physical properties: specific heat capacity, density, thermal conductivity
Chemical properties: kinetic parameters reaction enthalpy

→

Container

Shape, container material and thickness
Surroundings: heat transfer coefficient and emissivity

→

Simulations

For user-defined temperature program: isothermal, dynamic heating, multiple steps, modulated, external temperature profile

→

Visualization

2D/3D/Heatmap for temperature, conversion, conversion rate, concentrations, T_g for curing

Reactant

Physical properties:
specific heat capacity, density, thermal conductivity
Chemical properties:
kinetic parameters reaction enthalpy

The chemical properties of the reactant contain the reaction enthalpy and kinetic parameters from both model-free and model-based analysis. The model under consideration could be a comprehensive model that encompasses all reaction steps and their kinetic parameters. These parameters may include the activation energy, pre-exponential factor, reaction order, and parameters for autocatalysis.

These parameters can be retrieved from the Kinetics Neo software through the analysis of experimental data as presented in figure 1. It is possible to load a kinetic model with parameters into Termica Neo from a Kinetics Neo project with minimal effort.

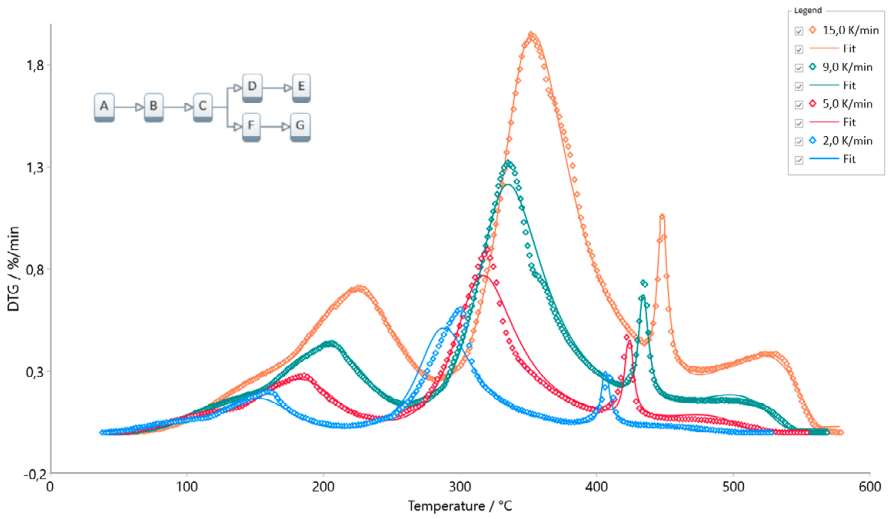


Figure 1. Complex kinetic models for the decomposition of ammonium paratungstate tetra-hydrate obtained in Kinetics Neo software can be easily opened for future simulations.

A reactant's physical properties encompass its specific heat capacity, density, and thermal conductivity, which are temperature-dependent.

The software contains the **Material Library** with the most frequently used reactants of different types. The physical properties of the reactant or container can be selected from the pre-installed Material Library or defined by the user (figure 2).

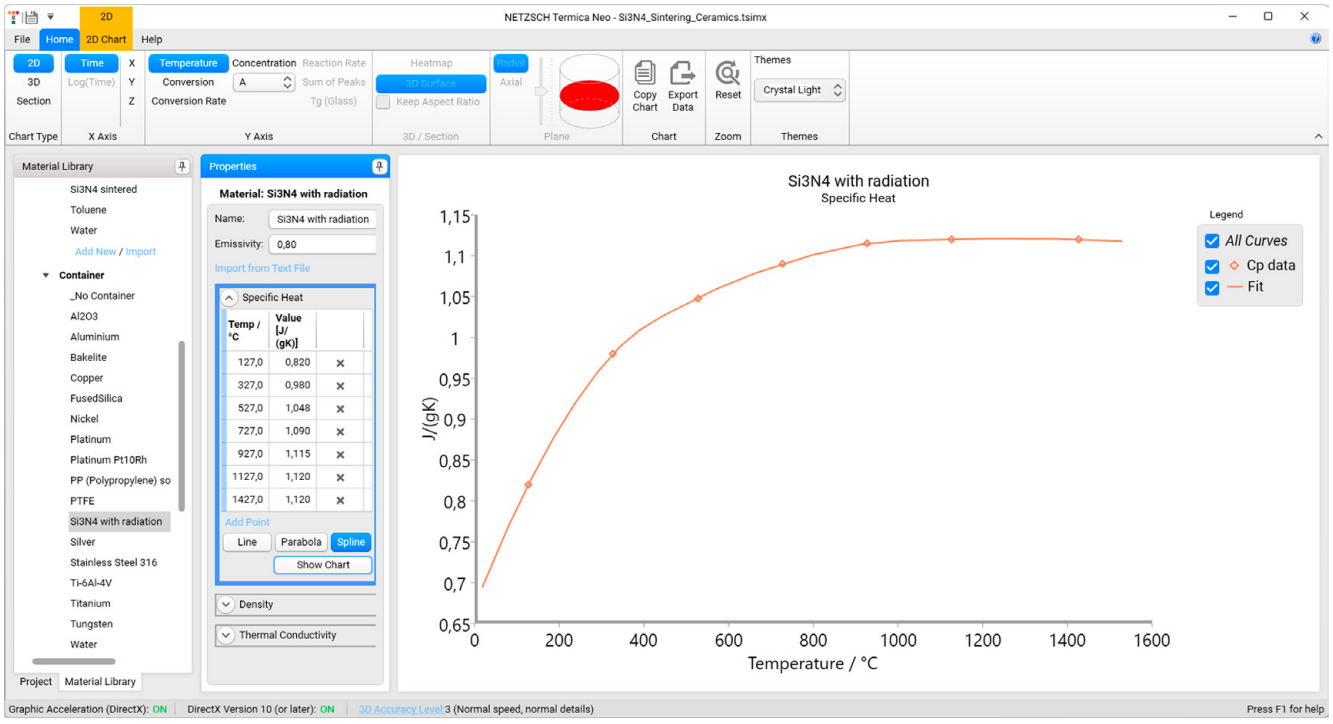
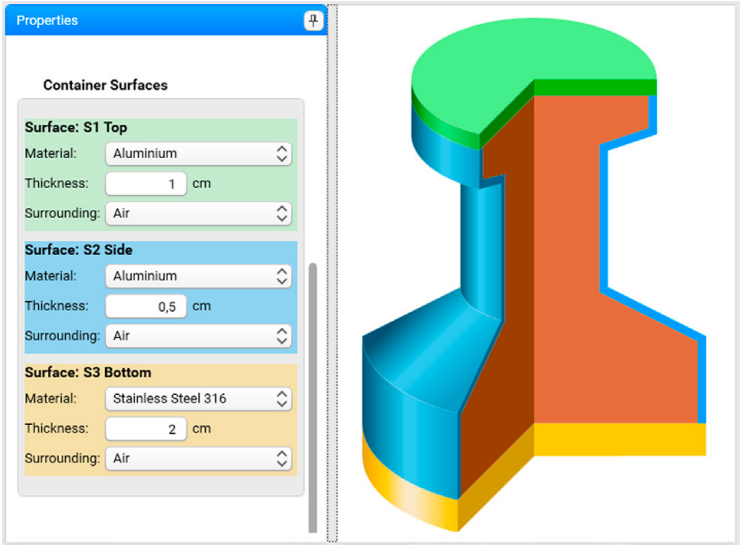


Figure 2. Temperature-dependent physical properties of reactants, container materials and surroundings in Material Library

Container

Shape, container material and thickness
Surroundings:
heat transfer coefficient and emissivity



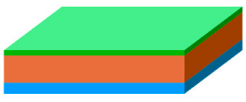
The reactant can be placed into a container of various shapes and made of different materials. Containers can possess geometries characterized by surfaces of varying thicknesses. It is possible to assing a distinct material to each surface within the container.

The physical properties of container materials can be selected from a pre-installed Material Library or defined by the user.

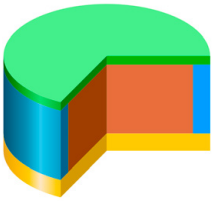
The Material Library contains a wide array of container materials, ranging from metals to heat-insulating materials, with their temperature-dependent physical properties and emissivity coefficient. For surrounding materials such as air or water, the Material Library includes the heat transfer coefficient on the surface.

Geometry of Standard Containers

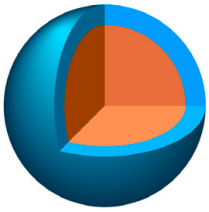
Infinite slab



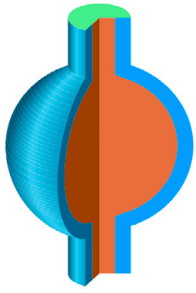
Cylinder



Sphere



Rotation shape with arbitrary profile



The surrounding media can be individually delineated for each surface. For illustration purposes, one might consider a scenario where the bottom surface is composed of concrete, while the top surface is in contact with air.

Simulations

For user-defined temperature program: isothermal, dynamic heating, multiple steps, modulated, external temperature profile

The simulation necessitates the establishment of specific temperature conditions. First, the initial temperature for the reacting volume and the ambient temperature conditions must be set. It is important to note that the surrounding temperatures may be different for different surfaces of the container:

- Isothermal
- Dynamic: constant heating or cooling rate
- Multiple step: sequence of dynamic and isothermal segments
- Step-iso: alternating segments of isothermal type and vertical jump
- Modulated isothermal
- Modulated dynamic
- External temperature profile: continuous temperature change

As illustrated in figure 1, the temperature data for epoxy curing at specific time points (46, 97, 153, 176, and 184 minutes) is presented as a function of the vertical section of the cylinder.

Termica Neo also offers the ability to save the simulated process as an AVI video (figure 2) for temperature, degree of curing and curing rate.

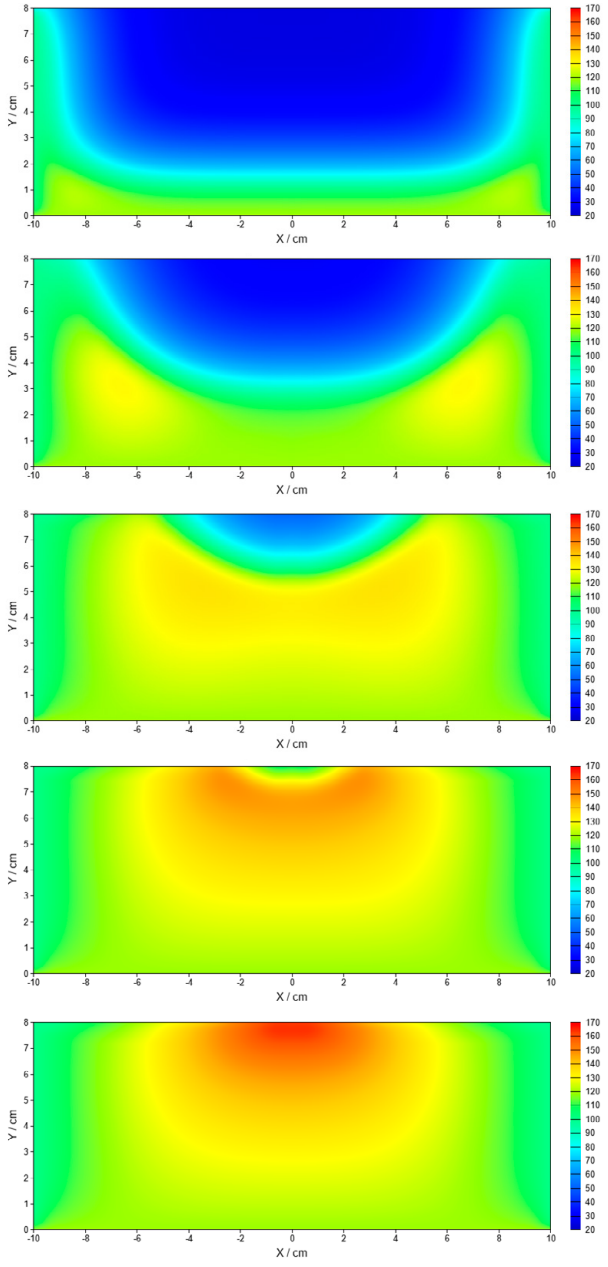


Figure 1: Curing of an epoxy resin in a cylinder; vertical section at specific time points

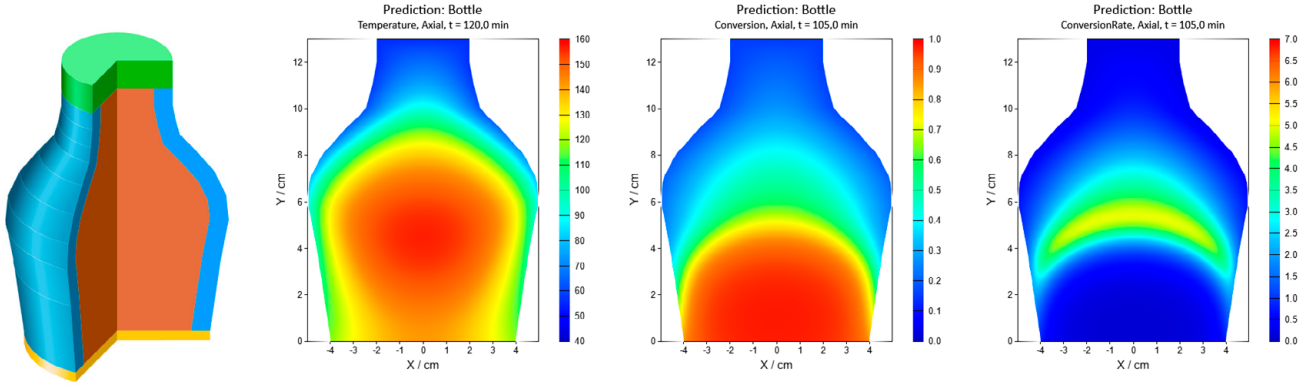


Figure 2: Excerpt of the simulation captured in an AVI video

Visualization

2D/3D/Heatmap
for temperature,
conversion,
conversion rate,
concentrations,
T_g for curing

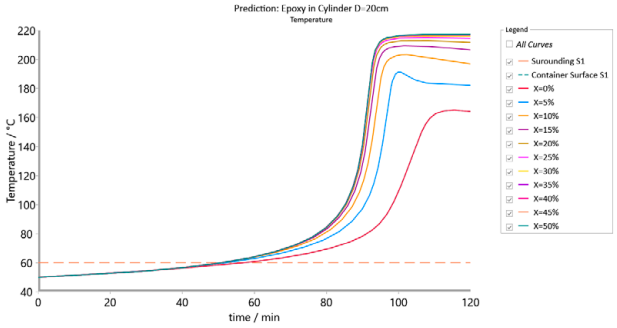


Figure 1A. 2D chart: Temperature vs. time at different coordinates

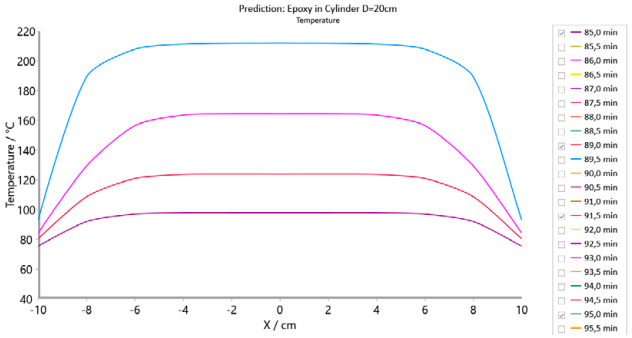


Figure 1B. 2D chart: Temperature vs. coordinate at different time points

Two-dimensional charts present the dependences of temperature on time at different coordinates (figure 1A) or on coordinate at different time points (figure 1B).

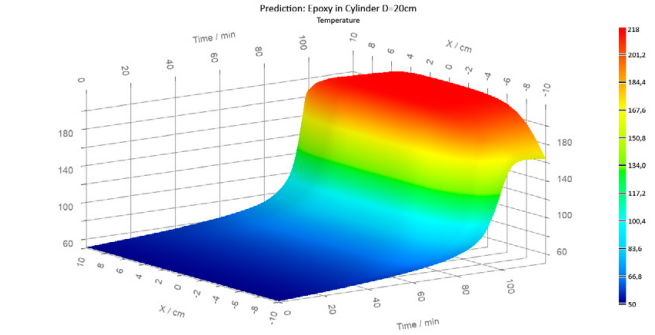


Figure 2A. 3D chart: Temperature vs. time and one coordinate

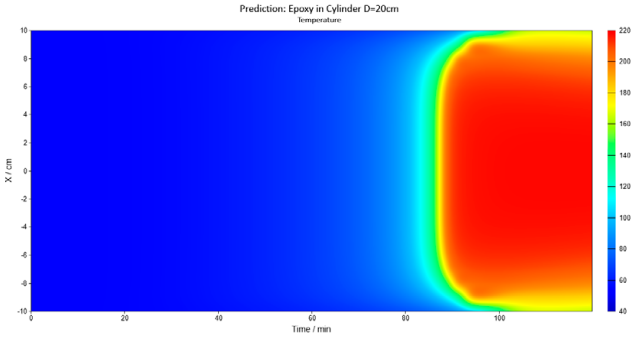


Figure 2B. Heatmap: Temperature vs. time and one coordinate

Three-dimensional diagrams for time and coordinate (figures 2A, 2B) or for two coordinates (figures 3A, 3B) can be presented as the surface (figures 2A, 3A) or as a heatmap (figures 2B, 3B).

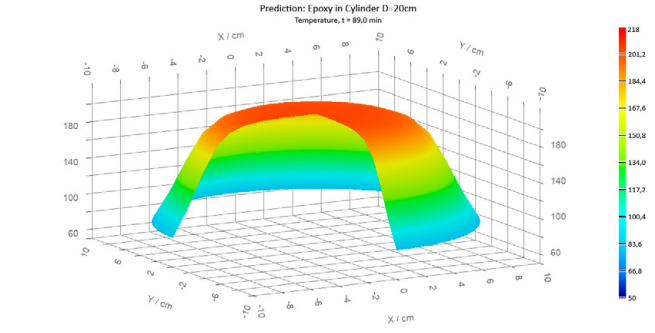


Figure 3A. 3D chart for selected cross-section: Temperature vs. two coordinates at the selected time point. Video is possible.

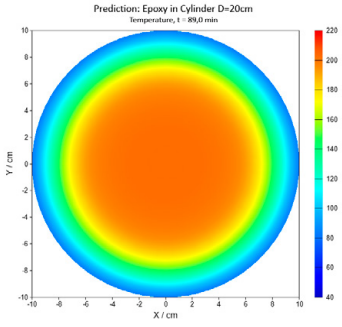


Figure 3B. Heatmap for selected cross-section: Temperature vs. two coordinates at the selected time point. Video is possible.

Three-dimensional charts can be customized through a series of mouse-driven actions, including rotation and zooming (see figures above). In Termica Neo, these types of result presentation are all implemented for temperature, conversion, conversion rate and the concentrations of all reactants and products, including intermediate reactants.

Applications

Simulating Epoxy Curing with Exothermal Heat Effects

The exothermal curing process causes the material to self-heat, leading to internal temperature gradients. We simulate the curing of an epoxy in cylindrical aluminum containers with varying wall thicknesses (0.3 to 1 cm) under controlled thermal conditions: 120°C at the bottom, 100°C on the sides, and 25°C at the top. This simulation determines whether complete curing occurs throughout the volume after 130 minutes (figure 1).

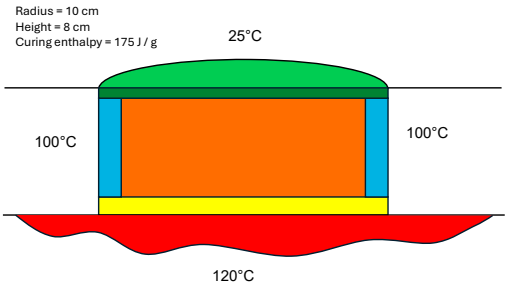


Figure 1: The simulation of curing is based on an aluminum container under the given conditions.

Simulation Results: Temperature Distribution

In figure 2, the simulation illustrates how temperature evolves over time along the vertical axis and radially at 66% of the cylinder's height. Due to the exothermal reaction, the material self-heats, resulting in a higher temperature at the center compared to the surrounding areas. At 130 min, temperature distributions are shown for both a vertical cross-section and a horizontal slice taken at 66% of the cylinder height, providing a clear view of thermal gradients during curing. The lower and central regions of the epoxy volume attain significantly elevated temperatures, whereas the top-center portion of the cylinder remains comparatively cool due to limited heat conduction and surface cooling (figure 3). The temperature plots reveal localized hot spots (red) resulting from the exothermal nature of the curing reaction. A prominent thermal peak is observed at approximately 4 cm in height and 6 cm radially from the cylinder wall, indicating a zone of intensified self-heating within the bulk material.

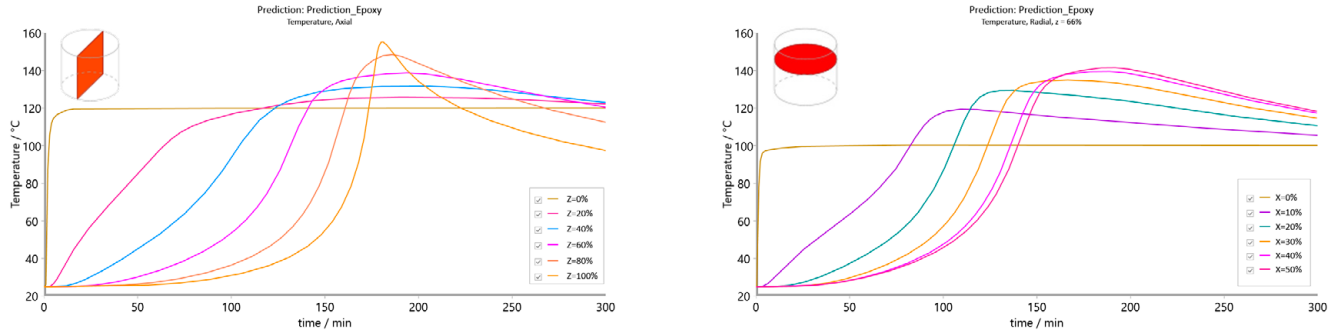


Figure 2: The simulation of the temperature in vertical and radial direction within the cylindrical container.

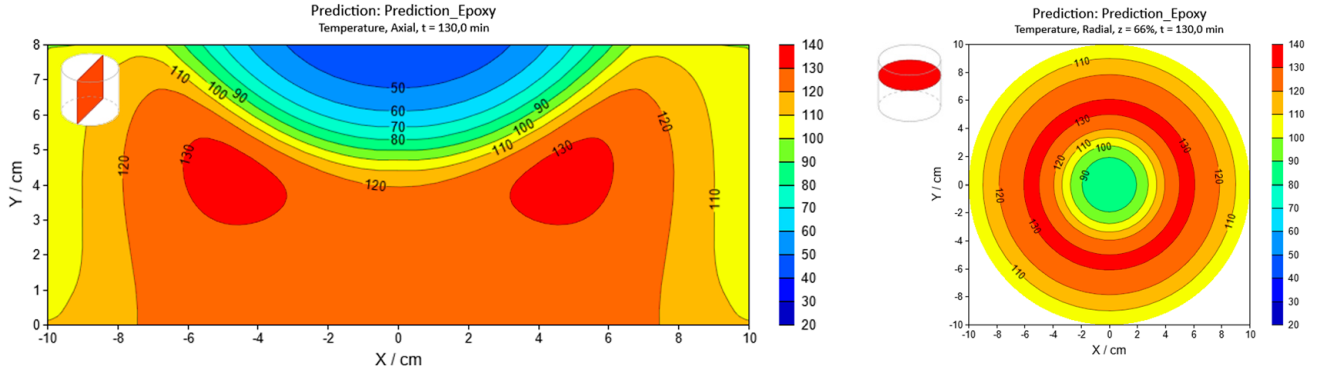


Figure 3: The temperature distribution of the vertical and horizontal sections in the cylinder at t=130 min.

Simulation Results: Conversion Rate

The distribution of the conversion rates is presented at a time of 130 min for both the vertical and horizontal cross-sections, with the data obtained at 66% of the cylinder's height (figure 4).

The reaction front propagates from the thermally heated bottom surface to the colder upper surface, driven by the thermal gradient. The regions indicated by red correspond to the highest observed reaction rates. The blue area, situated beneath the reaction front, signifies that the material has already undergone the curing process and the reaction has reached its completion. The blue area above the reaction front indicates that the material has not yet undergone the curing process

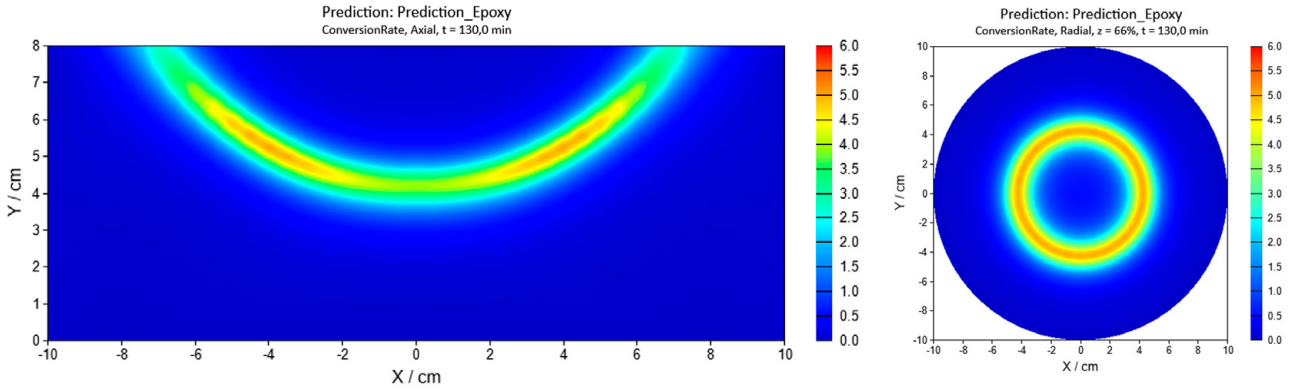


Figure 4: Simulation of the distribution of the conversion rate within the container.

Simulation Results: Degree of Conversion

Figure 5 indicates the degree of conversion for the horizontal cross-section at 50% of the sample height and a time of 130 min. The blue region in the center of the image indicates a low degree of cure near the vertical axis. The red regions, which indicate the maximum radius, signify completion of the curing process along the lateral surfaces.

The software facilitates the visualization of the cross-section at a user-selected vertical position within the cylinder.

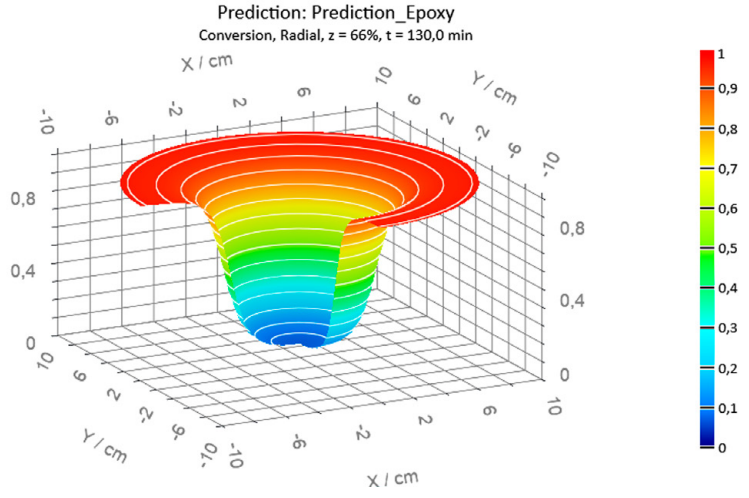


Figure 5: Simulation of the degree of conversion.

Glass Transition Temperature in the Curing Process

When a glass transition occurs during the cross-linking of a thermoset polymer, the reaction separates into domains dominated by different mechanisms. Far above the glass transition, the chemical reaction is fast and can be described by the Arrhenius relation. Near the glass transition, curing slows due to diffusion control. Below the glass transition temperature, the material vitrifies and the curing process slows down significantly.

This is why the kinetic model must be expanded with special diffusion control algorithms to account for the change in curing mechanisms.

Simulation Results: Temperature

The material temperature, T, which was measured at the 150-minute mark, was used to determine curing with diffusion control for both the radial and axial cross-sections (figure 1).

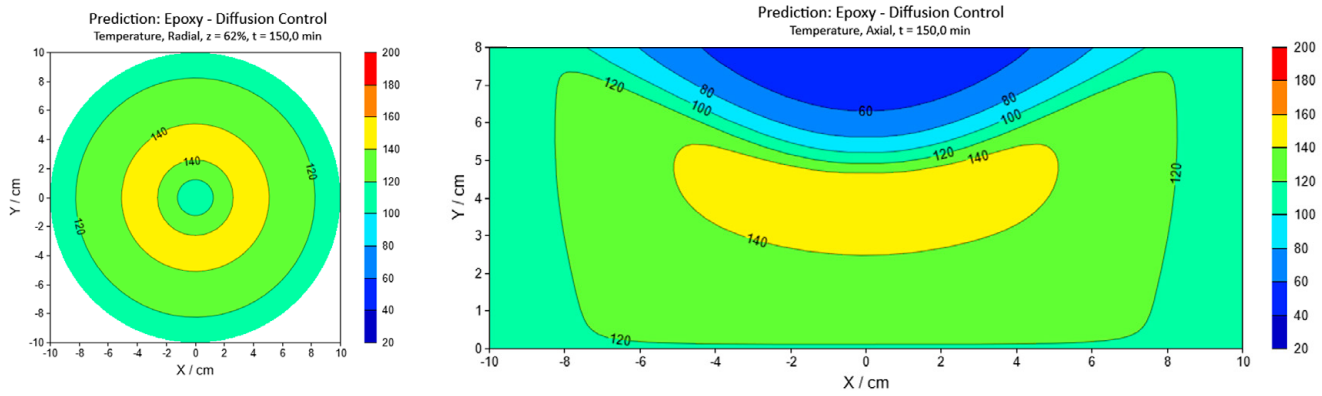


Figure 1: The simulation of the temperature at 150 min in radial and axial cross-section.

Simulation Results: Glass Transition Temperature

The prediction of the glass transition temperature (T_g) at 150 minutes is shown for both the radial and axial cross-sections, taking curing with diffusion control into account (figure 2).

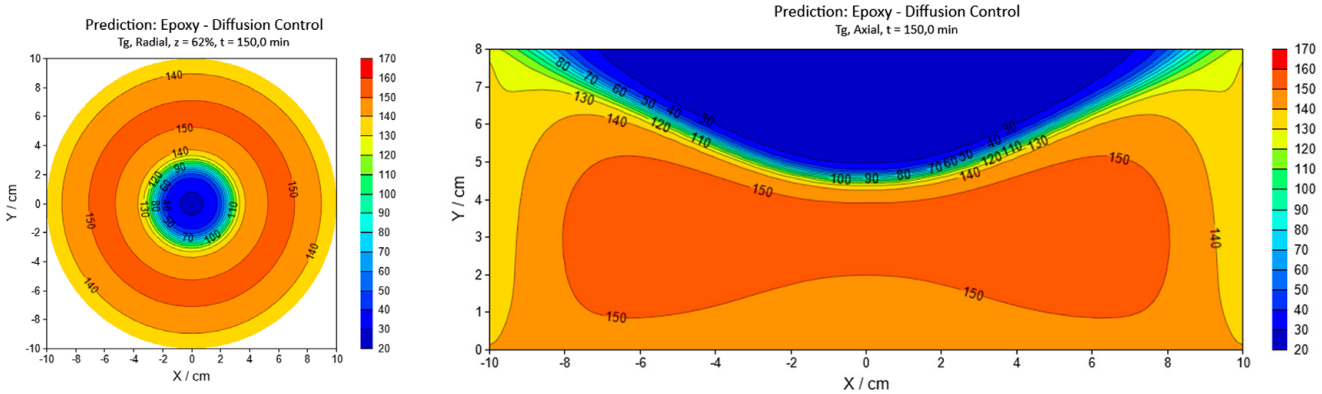


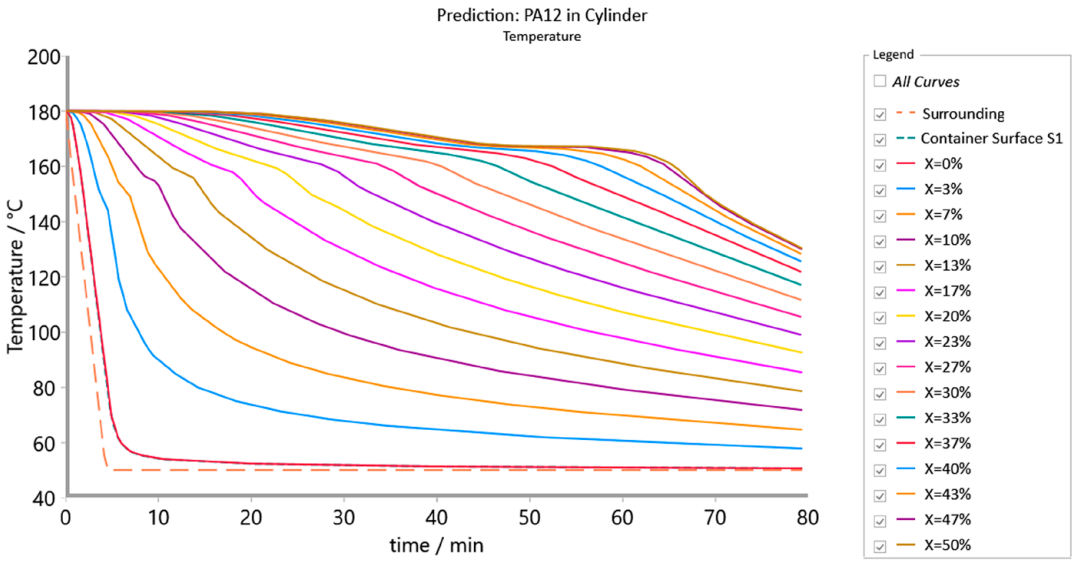
Figure 2: The simulation of the glass transition temperature.

If the current glass transition temperature, T_g, is below the current material temperature, then material is elastic/viscose, otherwise the material is vitrified and is in a glassy state.

Crystallization of PA 12 in a Cylinder

In the context of industrial manufacturing processes, such as injection molding or additive manufacturing (e.g., selective laser sintering [SLS]), it is imperative to understand the dynamics of crystallization rates and the subsequent degree of crystallinity. Accurate knowledge of these parameters is essential for ensuring the quality of the material during processing, as they directly impact the resulting product's physical and mechanical properties.

As illustrated in the figure, the simulation model demonstrates the crystallization process of PA12 within a cylinder rod with a diameter of 10 centimeters. The surrounding temperature undergoes a rapid decrease from 180°C to 50°C, subsequently stabilizing at a constant level. The surface temperature undergoes a rapid decrease, while the temperature in the center exhibits a slow decline. The exothermal effect of polymer crystallization manifests as a wave on the temperature curves between 150°C and 170°C. In those regions, where the cooling rate is faster, crystallization occurs at a lower temperature.



Prediction of the crystallization behavior within the cylinder rod

Protein Denaturation

A kinetic model of protein denaturation was created using the Kinetics Neo software based on differential scanning calorimetry (DSC) measurements. This model is used to simulate the denaturation process of a protein in an egg when immersed in boiling water. The egg was exposed to 100°C for eight minutes, then transferred to air at 25°C.

This simulation shows that the protein denaturation continues in the middle of the egg in air. The simulation presents the temperature (figure 1) and degree of denaturation (figure 2) as a section map after 4 minutes and as the function of time at different radial distances at an egg height of 50%.

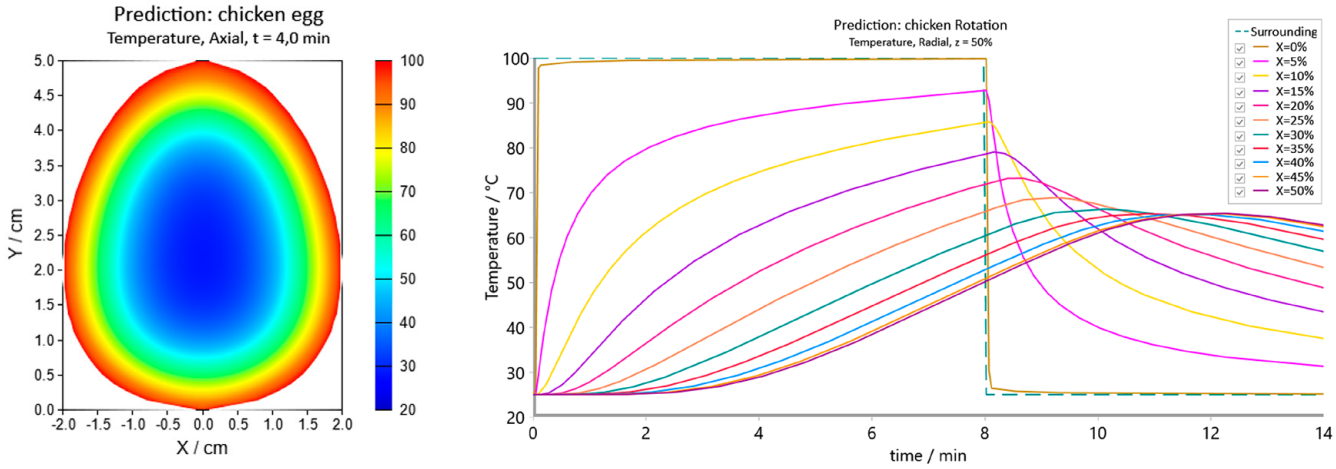


Figure 1: Simulation of the temperature in vertical cross-section and radial direction.

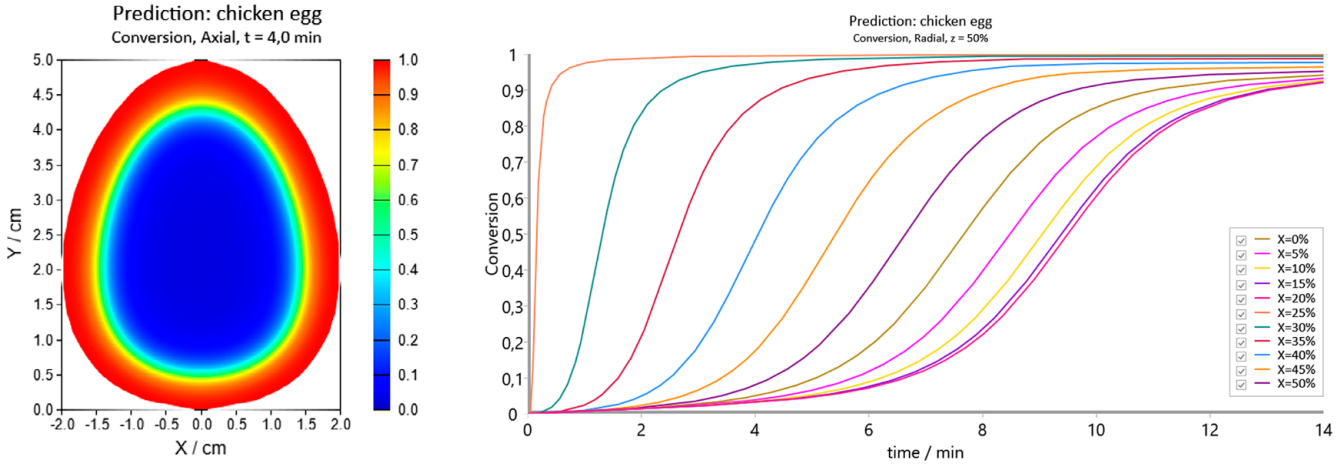


Figure 2: Simulation of the conversion in vertical cross-section and radial direction

Processes with Densification

Sintering of Ceramics, Consolidation in Polymers and Composites

Densification, consolidation, and sintering can lead to changes in a material's length or dimensions, often in the form of shrinkage or expansion.

Ceramic firing has specific features that must be considered during sintering. At high temperatures, thermal radiation becomes the main mechanism of heat transport over the surface.

The main distinguishing feature is the fast change in physical properties during this process. It occurs because the physical properties of the green body differ from those of the sintered material.

The density of the initial reactant differs from that of the final product. These changes in such materials as ceramics can be observed by means of dilatometry. During heating, silicon nitride (Si_3N_4) experiences a 17% decrease in linear size (length), which corresponds to an increase in density of more than 40% during the sintering process.

However, the thermal conductivity also changes significantly during the sintering process. For the green silicon nitride body, the thermal conductivity at 25°C amounts to 0.5 W/(m·K); for the sintered ceramic, it is 13 W/(m·K) – more than 25 times higher (figure 2).

High-Tech Ceramics: Si_3N_4 Simulation

In this example, the main sintering occurs between 50 and 60 minutes. At the same time, thermal conductivity increases. This results in low-temperature gradients in the ceramic part and a smaller temperature difference between the center and the surface (figure 1).

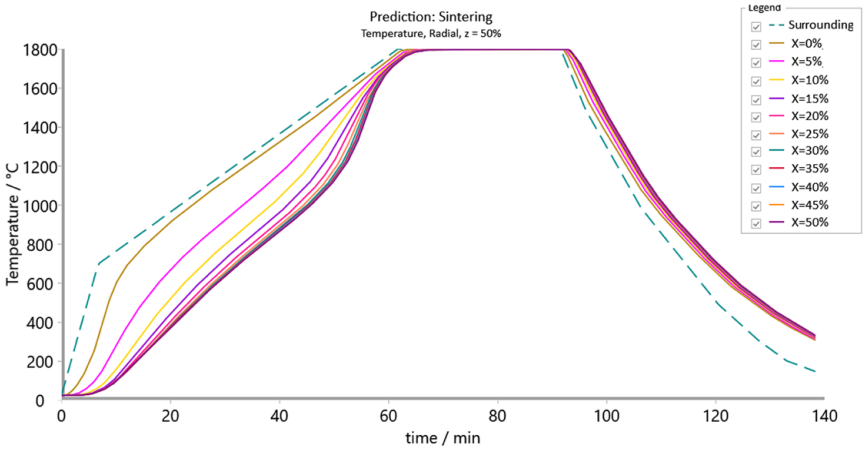
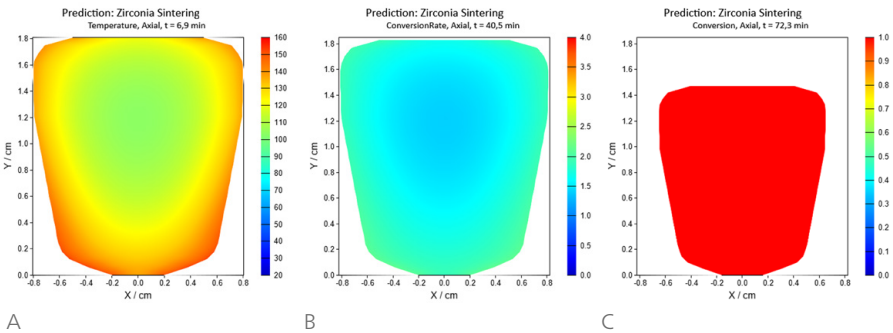


Figure 1: Radial temperatures of a ceramic for half-height of cylinder shape with diameter D = 10 cm and height H = 5 cm.

Dental Ceramics: Zirconia Firing

Zirconia ceramics are widely used in dental applications due to their excellent mechanical strength, biocompatibility, and aesthetic appeal. Figure 2 presents the simulation of the sintering process in zirconia ceramics with real-size geometry, allowing accurate predictions of the temperature distribution and shrinkage during firing. Figure 2A illustrates the temperature distribution at t = 6.9 min in the ceramic body. The sintering rate at time = 41 min (figure 2B) is higher at the surface than at the center, depending on the coordinates. Figure 2C presents the degree of sintering after an optimized firing cycle of 72 minutes, where the red color and the decreased linear size mean complete sintering.



A B C

Figure 2: Simulation of a dental ceramic for an optimized temperature profile. Vertical cross-sections for the temperature distribution at t = 6.9 min (A), conversion rate at t = 40.5 min (B), and degree of sintering at t = 72.3 min (C).

Concentrations for Multi-Step Processes

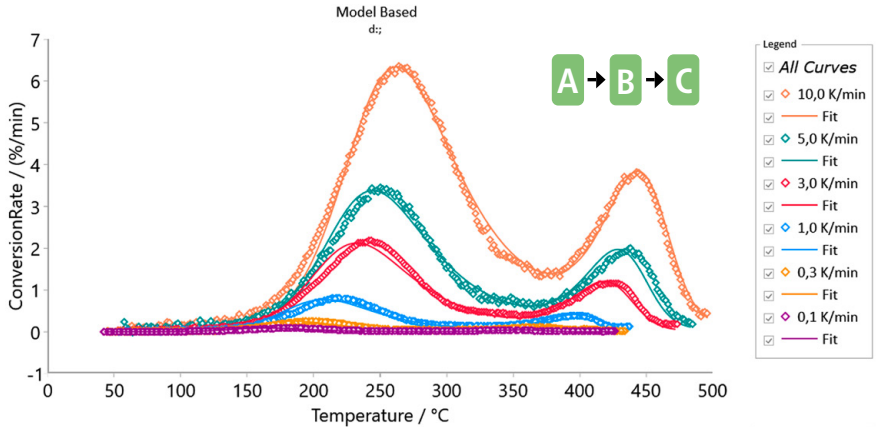


Figure 1. Kinetic model for a two-step decomposition process.

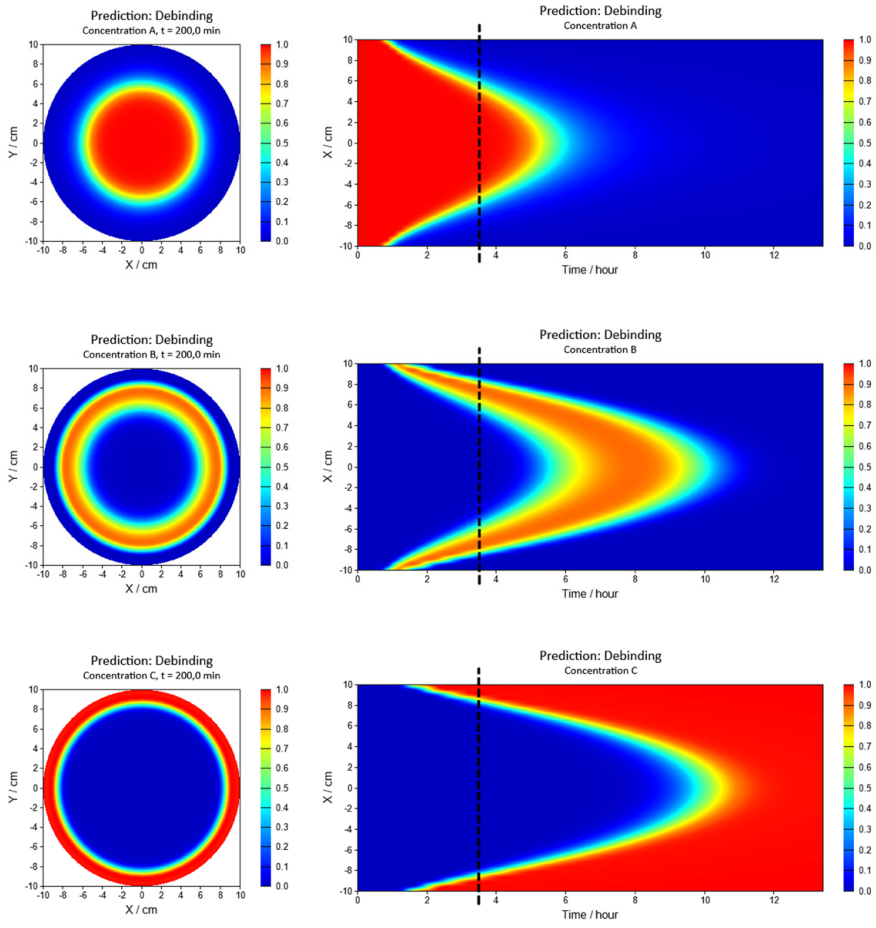


Figure 2: Prediction of the concentration levels of A, B, and C (left); and over time (right).

In multi-step reactions, the concentrations of intermediate and final reactants influence the mechanical and electrical properties of the final product. In order to achieve the homogeneous properties in the reacting volume, the distribution of all the reactant concentrations must be known.

This example illustrates a two-step kinetic model A → B → C with three reactants A, B and C (figure 1). Simulation of the two-step reaction in a cylindrical volume presents the concentrations of all three reactants at selected time points.

The rectangular plots in figure 2 show the time-dependent concentration at various radial points. The dashed line represents the time = 200 min, at which point the round cross-sections of cylinder are taken. Multi-step kinetic products contain the initial reactant, the final product, and the intermediate reactants, which are important for some industrial applications.

Safe Storage of Highly Energetic Materials

When predicting about the storage or transportation of highly energetic materials in the chemical industry, the temperature gradients in the reacting medium must be considered. For highly exothermal reactions, areas with higher temperature and faster reactions feature more intensive heat production and self-heating. Such local areas then become hotspots where runaway or thermal explosions can begin.

Accelerating Decomposition Temperature (SADT) – AIBN

The Self-Accelerating Decomposition Temperature (SADT) is the lowest ambient temperature at which a self-reactive substance will decompose in a specified commercial package within a week or even less. Above SADT, the reaction rate becomes so rapid that the heat generated outpaces the heat removal rate from the package, leading to a self-sustaining reaction. Specifically, SADT is defined as the lowest ambient temperature at which the material temperature exceeds the ambient temperature by 6K after 7 days, after having started 2K below ambient temperature.

The NETZSCH software Termica Neo provides time-dependent and temperature-dependent results for the temperature, the concentration of all reactants and the reaction rate in 2D and 3D view. It is also possible to search for the self-accelerating decomposition temperature (SADT) as well as simulate adiabatic conditions and infinite heat transfer to the surroundings.

The following example demonstrates the simulation of a 50-kg cylindrical package of azobisisobutyronitrile (AIBN) in air.

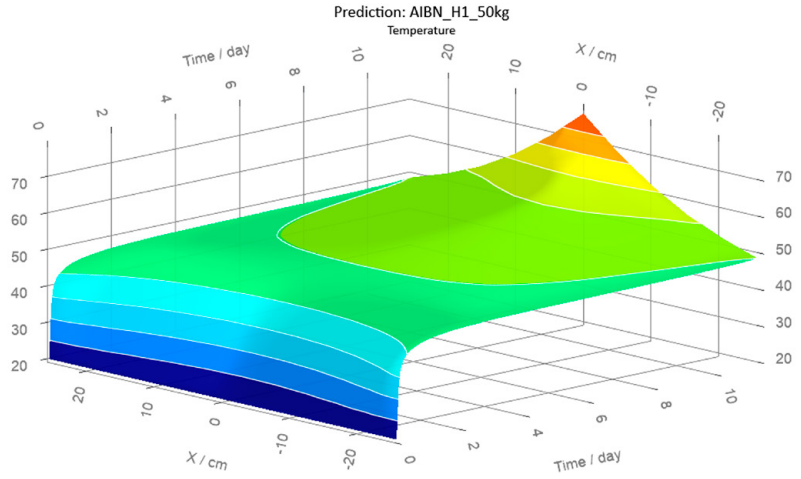


Figure 1: SADT calculation for the decomposition of the package of 50 kg of AIBN.

Simulation Results: Temperature

The temperature (x,t) is shown for the decomposition of the package of 50 kg of AIBN. A cylindrical package (room temperature in air) with an initial diameter of 50 cm is placed under storage at a temperature of 48°C (figures 1 and 2).

Verification of this simulation can be found in Thermochimica Acta 621(2015) 25-35.

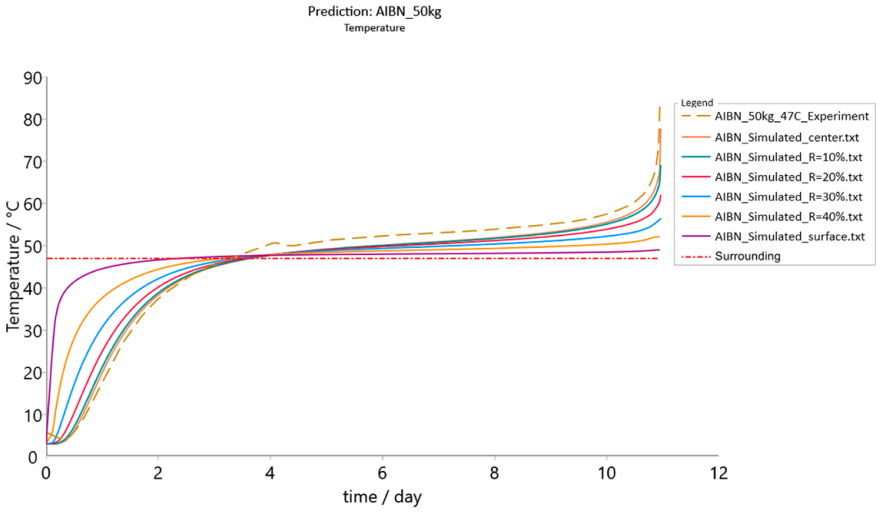
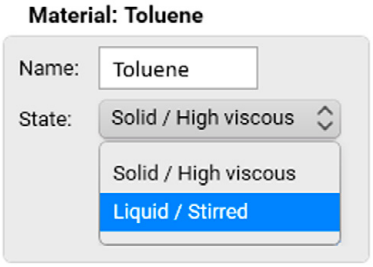


Figure 2: Prediction of the temperature progression for a cylindrical package at different radial distances, depending on time; the dashed curve is the experimental data measured in the center.

Decomposition of 20% DTBP in Toluene

In chemistry, DTBP (di-tert-butyl peroxide) in toluene refers to a solution of di-tert-butyl peroxide, a reactive organic peroxide, dissolved in the solvent toluene. DTBP is a radical initiator, meaning it generates free radicals upon thermal decomposition, making it useful in various chemical reactions and processes like polymerization.

Simulations in Termica Neo can be carried out for both solid and liquid materials. Liquids are assumed here to have high convection or stirring. Therefore, liquids have a uniform temperature without gradients.



Simulation in Liquids

The simulation was calculated for a liquid solution of 20% di-tert-butyl peroxide (DTBP) in toluene in an 8.5-ml titanium container with a radius of R = 2.5 cm and a wall thickness of 0.89 mm (figure 1).

The simulation results were confirmed by accelerating rate calorimetry measurements using the NETZSCH ARC 244 (figure 2).

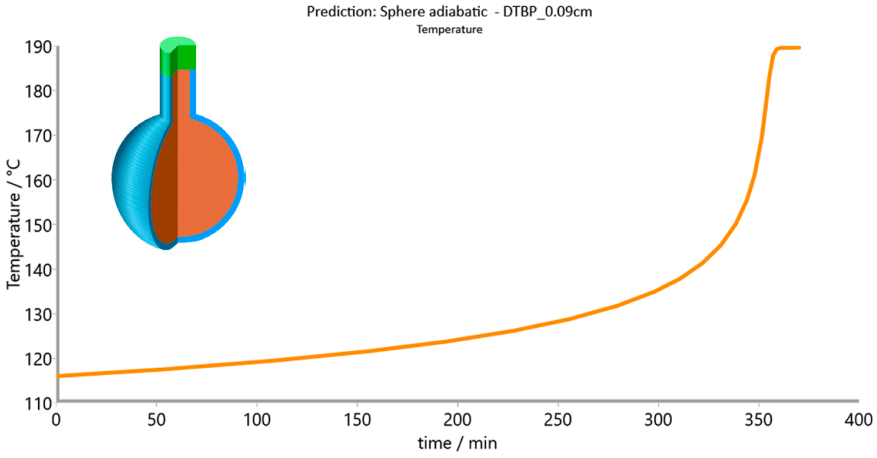


Figure 1: Prediction of the temperature progression.

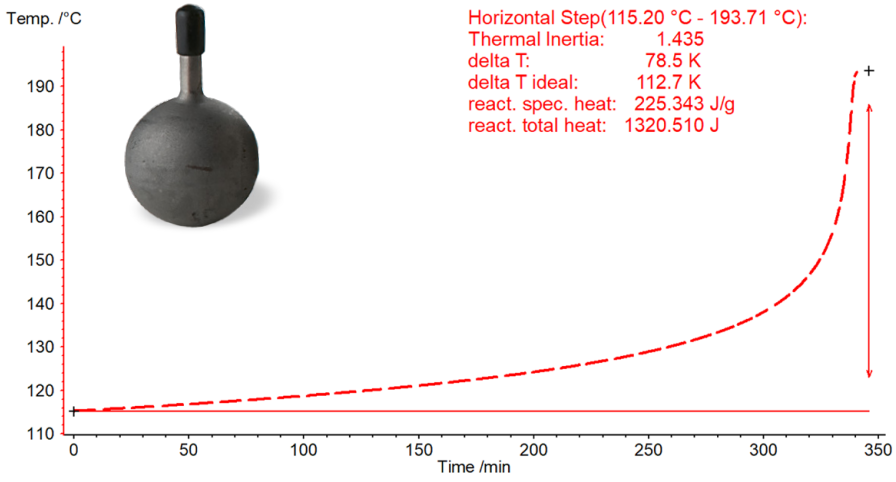


Figure 2: Confirmation of the simulation by means of an ARC 244 measurement.

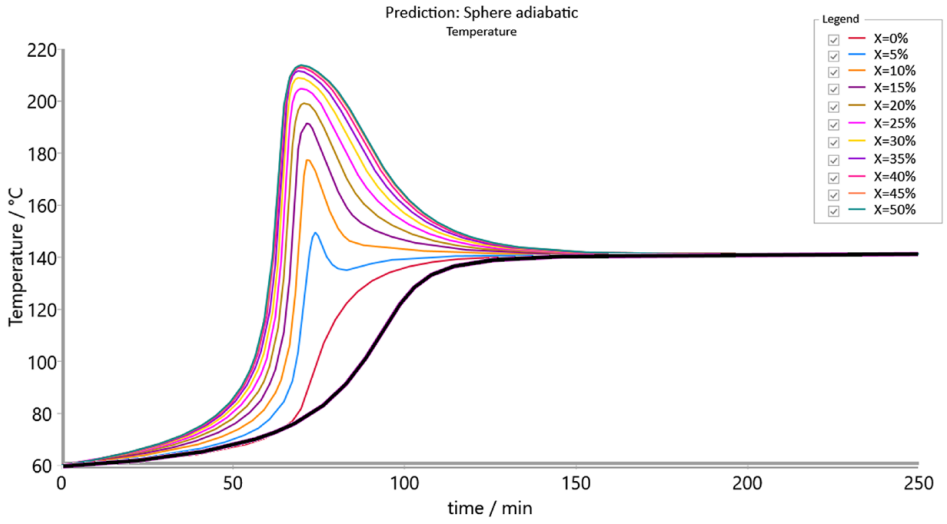
Reactant in an Adiabatic Container

Adiabatic simulations for liquids and solids involve modeling systems where no heat is exchanged with the surroundings. These simulations are crucial for understanding various phenomena, including phase transitions, material properties, and energy storage. However, these investigations also show that adiabatic simulations for liquids and solids yield different results.

The temperature of low-viscous liquids with convection or stirring is uniform (black curve). The reactant has no temperature gradients, and it heats up very slowly. It is usually calculated according to the factor of thermal inertia, Phi (see figure below).

Exothermal reactions in solids lead to temperature gradients and overheating in the center, where heat accumulates. Solids heat up faster, have a lower Time to Maximum Rate (TMR), and have a higher maximum temperature (colored curves in the figure). Therefore, calculation for solids according to the Φ-factor is inaccurate and dangerous.

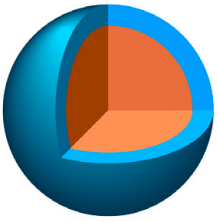
The simulation for solids, here demonstrated as the prediction, clearly shows an earlier reaction at a higher temperature than the calculation according to the Φ-factor. The final temperature for both simulations is the same and corresponds to the heat balance.



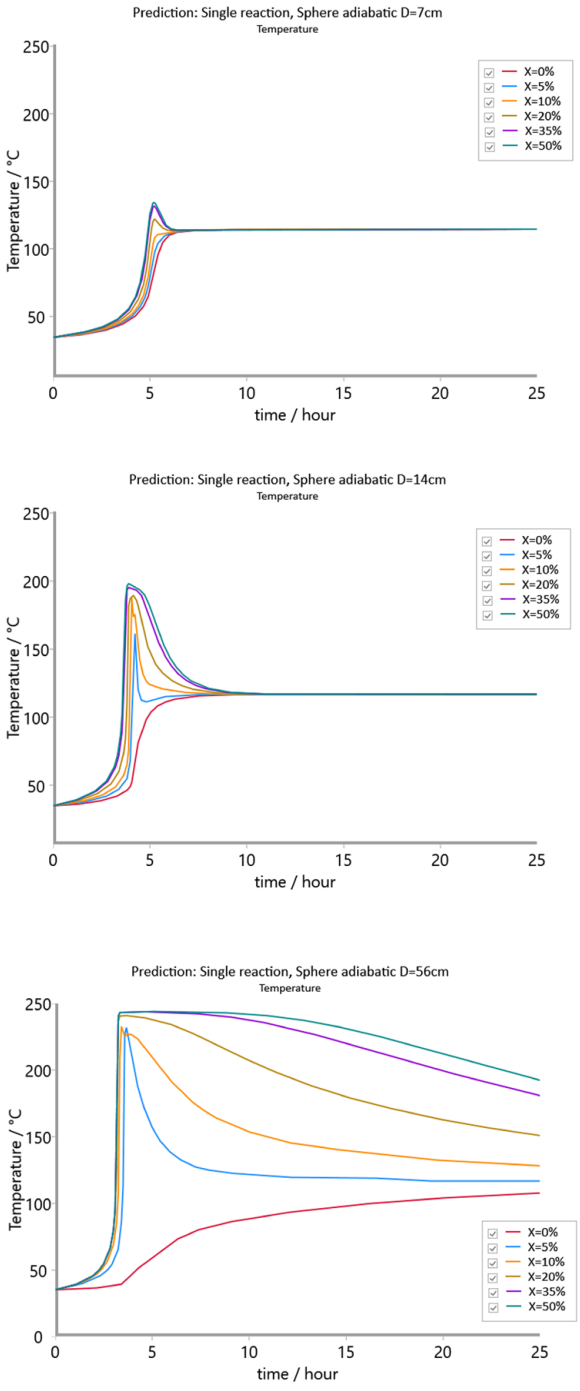
Simulation of the temperature distribution in an adiabatic system: solid reactant (colored curves), and liquid reactant (black curve).

Adiabatic Scale-Up for Single Reaction

The temperature of the material under adiabatic conditions for 24 hours is very important for the safety of industrial reactions with high exothermal effect. For liquid materials with stirring the temperature in the reacting volume is uniform and simulation can be carried out according to the factor of thermal inertia, Phi, which is the ratio of the heat capacity of the material with container to that of the material alone. However, knowledge of the Phi-factor only is not enough for simulation of the correct temperature distribution.



The figure displays the simulations under the assumption of a single reaction for three different diameters. In the first simulation, with D = 7 cm, there are almost no temperature gradients or overheating. The second simulation, with D = 14 cm, exhibits a maximum overheating in the center. The third simulation, with D = 56 cm, has a maximum possible over-heating at the center, which corresponds to an adiabatic temperature increase for a pure material with a Phi-factor of 1. However, the final temperature is the same for all simulations, because of the heat balance with the same Phi-factor.



Simulations for single reaction, with reaction heat 395 J/g, Phi=1.4; diameters 7, 14 and 56 cm.

SIMULATIONS FOR THE DIFFERENT REACTING VOLUMES IN SOLIDS WITH THE SAME Φ-FACTOR LEAD TO DIFFERENT TEMPERATURE DISTRIBUTIONS.

Adiabatic Scale-Up for Primary and Secondary Reactions

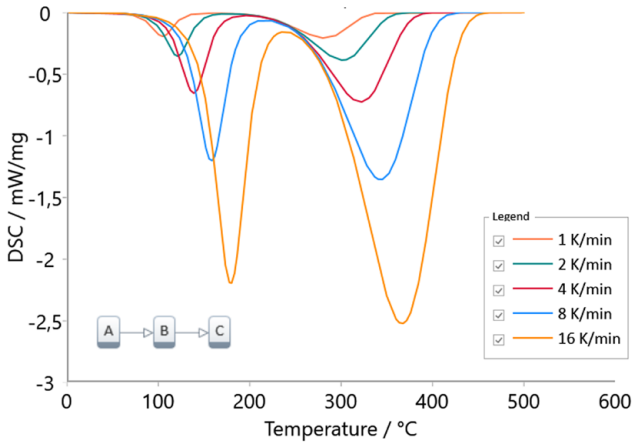


Figure 1: Example of a DSC measurement up to 500°C at different heating rates between 1 K/min and 16 K/min.

Many industrial applications have secondary decomposition reactions, which must be avoided during industrial processes. These highly exothermal secondary reactions may lead to serious damage if they get out of control. Therefore, it is important to know the temperature increase for adiabatic cases.

The current simulation example presents the adiabatic scale-up simulation over a 24-hour period for primary and secondary reactions in solids for the same Phi-factor.

Based on the DSC measurements (figure 1), three simulations are done for a Phi-factor of 1.4 (figure 2). After 24 hours, only the primary reaction is finished for the first two simulations, with D = 7 cm and D = 14 cm. The second simulation exhibits slight overheating in the center. In the third simulation with D = 56 cm, overheating in the primary reaction was too high, triggering the secondary reaction. The simulation shows that the larger the size, the greater the overheating in the center. The simulation helps determine the size at which overheating in the center becomes too high and leads to dangerous triggering of the secondary reaction.

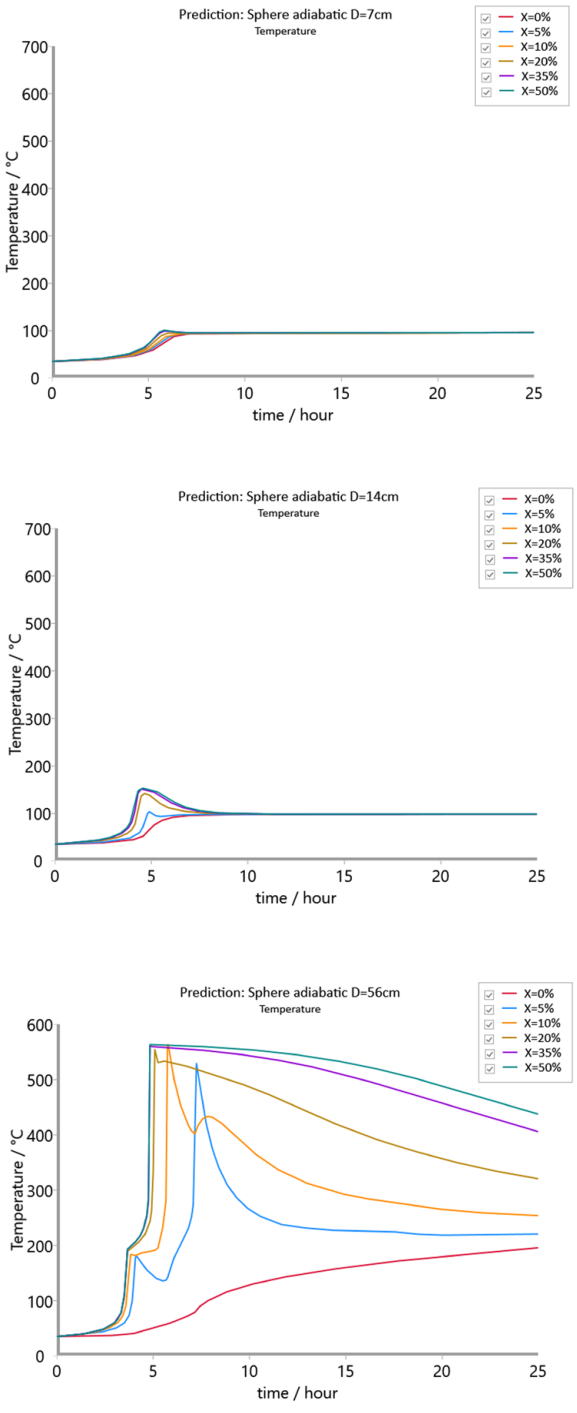


Figure 2: The primary reaction amounts to 300 J/g; the secondary reaction to 700 J/g; the Phi-factor for all simulations amounts to 1.4; diameters 7, 14 and 56 cm.

Key Technical Specifications

Highlights of Termica Neo – Simulation of the Thermal Behavior in Large Sample Volumes	
Purpose	Termica Neo is a software program designed for the simulation of thermal behavior and thermal safety of chemical reactions and crystallization in solids or liquids in volumes with characerizing size, ranging from centimeters to meters. The primary applications of this approach involve materials characterized by elevated thermal potential, in conjunction with reactions such as curing, cross-linking, sintering, decomposition, 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 reaction volume 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 temperature 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, such as the Self-Accelerating Decomposition Temperature (SADT).
System Requirements	
Prerequisites	Kinetics Neo version 2.5 or later
Operating systems	x64 versions of Microsoft Windows 11 or Windows 10
Integrated help	Context-sensitive, online help web site
Minimum hardware	Intel® Core i5 processor, 11th generation (Core i5 11400) or later, 16 GB RAM, DirectX 11 compatible graphics, display 1440x1050
Recommended hardware	Intel® Core i7 processor, 11th generation or later, 24 GB RAM, graphics nVidia 1080 GTX or better, display 1920x1200

Data for Simulation

Reactant

Kinetic parameters and equations are based on a previous kinetic evaluation and are loaded directly from the Kinetics Neo project; they include:

- Possible data type:
  - DSC
  - DSC with diffusion control
  - DTA
  - TGA
  - DIL
  - DEA
  - ARC Temperature
  - Viscosity
  - MS
  - DMA
- Analysis 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 enthalpy
- 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
  - Rotational body
- Material library with temperature-dependent physical properties for the container:
  - Specific heat capacity
  - Density
  - Thermal conductivity
- Surfaces:
  - The wall of each surface has its 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 coefficient
- Material library contains special surroundings:
  - Adiabatic (no 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

Simulations

Results

- Temperature T
- Conversion α
- Conversion rate dα/dt
- Glass transition temperature, T_g, for curing reactions with diffusion control
- Concentrations of individual reactants in multi-step reactions

Visualization of 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 with different spatial coordinates.
- Two-dimensional chart (for one-dimensional geometry): curves for T, α, dα/dt, concentrations, T_g as a function of spatial coordinates at any user-defined time point. Could be presented as the set of curves with different time values.
- Three-dimensional: surface for T, α, dα/dt, concentrations, T_g as a function of time and one selected spatial coordinate, where other spatial coordinates 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 coordinates 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
- Video of process in AVI format for cross-sections: both heatmap and three-dimensional surface

Graphical options

- Selection of the visual theme for user interface
- 2D chart
  - show/hide
    - legend
    - grid
    - zoom bars
  - select
    - legend font
    - axis font
    - axis thickness
- 3D chart
  - rotate 3D surface
  - show/hide
    - color surface
    - contour lines
    - wireframe
  - select
    - gradient/levels color palette
    - orthogonal/perspective projection mode
    - lighting and opacity effects
- Heatmap chart
  - show/hide
  - color surface
  - contour lines
  - grid lines
  - data points for polar plot
  - select gradient/levels color palette

AT A GLANCE

Advantages and Added Value of Termica Neo Software

1. Scale-Up Simulation

Accurately simulates thermal processes on large scales.
Facilitates a smooth transition from the lab-scale to industrial-scale productions.

2. Time and Cost Savings

Simulates and predicts thermal behavior without the need for extensive experimental trials at industrial scales.
Reduces time and resources required for physical testing.

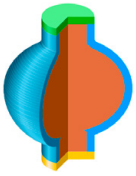
3. Precision and Control

Offers precise control over critical variables such as temperature, time, and concentration.
Enhances the ability to optimize and fine-tune processes for better efficiency.

4. Thermal Safety for Chemical Reactions (Storage and Transportation)

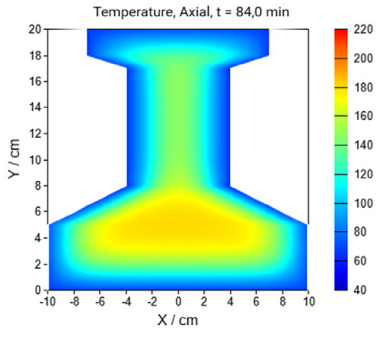
Ensures thermal safety of chemical reactions, enabling safe storage and transportation while predicting and decreasing risks of thermal runaway to prevent dangerous scenarios during storage and transport.

Shape

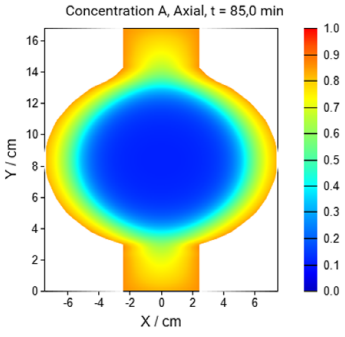


Shape

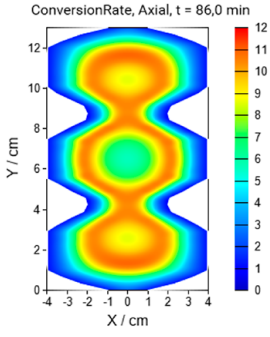
Shape



Temperature



Concentrations



Reaction 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.

Proven Excellence.

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