

AKTS Software



Advanced Kinetics

Thermokinetics, Thermal Safety,
Reaction Calorimetry, Migration Limits

What is AKTS software?

Designed by our long-term partner AKTS, Setaram uses their software ensuring a global solution for kinetic analysis, migration studies in packaging, and the determination of thermal safety.

AKTS software suite can be applied to the study of the thermal stability of substances, to the safety analysis of physical-chemical processes, and to the investigation of the safety and quality of packaged substances.



HIGHLIGHTS

Additional characteristics and behavior of materials

AKTS software provides a means of inferring additional characteristics and behavior of materials examined, based on conventional thermoanalytical measurements.

ACCURATE DETERMINATION

A key benefit of this software is the accurate determination of the thermal stability of products (shelf-life/transformation) for quantities, temperatures and time scales beyond those measured.

CRITICAL DATA INFORMATION

This provides critical data often difficult to obtain for reasons of time, cost and feasibility.

THERMOKINETICS SOFTWARE

Evaluation of Kinetic Parameters from Conventional Thermoanalytical Data

Thermokinetics software allows kinetic analysis from the conventional thermoanalytical data collected at any temperature mode using both iso-conversional and model-fitting approaches.

BENEFITS AT A GLANCE



Automatic baseline construction and use of the differential isoconversional method of Friedman (model free) for an advanced baseline optimization.



Standard procedure of **ASTM A698**.



Different types of baseline considered:

Sigmoid, Tangential Sigmoid, Linear Horizontal First or Last Point, Tangential and many more.



Prediction of the reaction progress and thermal stability of materials under any temperature mode.



Differential isoconversional method of Friedman (model free).



Integral isoconversional method of Ozawa-Flynn-Wall (model free).

THERMOKINETICS DSC-ARC

Quick evaluation of standard safety parameters TMRad and SADT

New method for the evaluation of hazard indicators based on merging Differential Scanning Calorimeter (or Calvet calorimeter) and Accelerated Rate Calorimeter measurements.

BENEFITS AT A GLANCE

A simple two-steps kinetic approach:



Determination of the **kinetic parameters** of the decomposition reaction for quantifying the heat release rate.



Application of the heat balance, for quantifying the heat loss rate on a **gram-, kilogram- and ton- scale**.



Determination of the Time to Maximum Rate **under adiabatic conditions** (typically TMRad 24h, with $\Phi=1$)



SADT determination according to **STANAG 4383** and **UN regulations** (Tests H.4 and H.1)

THERMAL SAFETY SOFTWARE

Evaluation of Safety Parameters TMRad, Safety Diagrams, Simulation of ARC and Runaway Reactions, Determination of SADT

Thermal Safety Software allows evaluation of safety parameters such as TMRad, construction of safety diagrams, simulation of ARC and runaway reactions, determination of SADT.

BENEFITS AT A GLANCE

Construction of a safety diagram: runaway time as a function of process temperature under adiabatic conditions ($TMRad = f(T)$).

ARC simulations, determination of the influence of the different Phi factors ($\Phi=1$ and $\Phi>1$) on the TMRad.

Determination of the Self-Accelerating Decomposition Temperature (SADT) according to the recommendations of Manual of Tests and Criteria of the United Nations on the transport of dangerous goods.

Automatic **determination of the starting temperatures corresponding to TMRad** of 7 days, 24h, 8h, and 4h.

THERMOKINETICS SPARSE DATA SOFTWARE

Evaluation of Kinetic Parameters from Sparse, Discontinuously Collected Thermoanalytical Data

Thermokinetics sparse data software allows kinetic analysis from the sparse data (20–30 experimental points) generally collected in isothermal temperature mode using advanced modelfitting and statistical approaches.

BENEFITS AT A GLANCE

Evaluation of kinetic parameters from sparse data (e.g. GC or HPLC data collected at three temperatures only).

S-shape **kinetic models** applied for **single or multiple reaction stages**.

Application of advanced statistics (Akaike and Bayesian information criteria) for kinetic model selection and ranking.

Bootstrap method for **evaluation of prediction bands**.

Possibility of **simulation of the reaction progress** after arbitrarily chosen aging time under any temperature profile.

SPECIFIC MIGRATION LIMITS SOFTWARE

Prediction of Migration Rate of Species from Packaging Materials to Packed Goods

Specific migration limits software allows the quantification and prediction of the migration rate of the packaging materials components into the packed items.

BENEFITS AT A GLANCE



Migration modeling with SML Software allows **the evaluation of the rate of the diffusion** of organic migrants present in the plastic multi-layer packaging into the packed items.



The application of SML Software ensures the **compliance** of plastic food contact materials and articles **with specific migration limits according to EU regulations and Swiss Legislation.**



SML allows the migration **simulations at any temperature mode.**



SML permits the evaluation of setoff and **subsequent setoff effects.**



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