



Advanced Kinetics and Technology Solutions

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**AKTS-Thermokinetics software - Thermal Aging and Thermal Safety Versions:  
EXAMPLE OFFER for One (1) license**

Pos	Description	Unit Price EUR	Qty	Total EUR
1	<p><b>AKTS-Thermokinetics Software - One (1) Thermal Aging License Version 3</b> (Upgrade: includes one (1) year subscription for free upgrade)</p> <p>Determination of kinetic parameters (activation energy <math>E</math> and pre-exponential factor in Arrhenius equation <math>A</math>) of complex multistage overlapped reactions based on multi-curves methods from HFC, DSC, nanoDSC, microDSC, C-80, DTA, TG and/or DTG, TG-MS, TG-FTIR measurements and prediction of the reaction progress and thermal stability of materials under any temperature mode.</p> <p>► <b>Advanced kinetic analysis :</b></p> <ul style="list-style-type: none"><li>• automatic baseline construction and use of the differential isoconversional method of Friedman (model free) for an advanced baseline optimization</li><li>• smoothing of data (Savitzky-Golay) and spikes correction</li><li>• differential isoconversional method of Friedman (model free)</li><li>• integral isoconversional method of Ozawa-Flynn-Wall (model free)</li><li>• standard procedure of ASTM A698</li><li>• model fitting method applying all commonly used equations for the description of the decomposition reactions e.g. n-th order reactions (Fn), nucleation (Avrami-Erofeev, An, A2, A1.5), diffusion (parabolic law D1, Valesi D2, Jander D3, Brounshtein D4) movement of the phase boundary (shrinking core model, Rn, R1, R2), autocatalysis</li><li>• calculations using any type of kinetic equation introduced by a user e.g. <math>d\alpha/dt = 1e10 * \exp(-100000/8.314/(T+273.15)) * (1-\alpha)</math> or <math>d\alpha/dt = A(\alpha) * \exp(-E(\alpha)/8.314/(T+273.15)) * (1-\alpha)</math></li></ul> <p>► <b>Prediction of the reaction progress and thermal stability of materials under any temperature mode:</b></p> <ul style="list-style-type: none"><li>• isothermal and non-isothermal, stepwise</li><li>• modulated temperature or periodic temperature variations</li><li>• rapid temperature increase (temperature shock)</li><li>• real atmospheric temperature profiles for investigating properties of e.g. low-temperature decomposed substances under different climates (yearly temperature profiles with daily minimal and maximal fluctuations. 50 climates available in the default version).</li><li>• NATO norm STANAG 2895 temperature profile: Zones A1, A2, A3, B1, B2, B3, C0, C1, C2, C3, C4, M1, M2, M3.</li></ul> <p>customized temperature profiles: possibility to compare the reaction progress of substances at any temperature profile</p> <ul style="list-style-type: none"><li>• combination of mass loss TG, heat flow signal e.g. DSC/DTA and MS data in multi-projects for simultaneous comparison of the mass loss, heat flow and volatiles species evolution at any temperature profile</li><li>• confidence interval of the prediction</li><li>• viewing data in form of overall conversion <math>\alpha(T(t))</math>, <math>d\alpha(T(t))/dt</math></li><li>• viewing data in natural form <math>Q(T(t))</math>, <math>dQ(T(t))/dt</math>, <math>P(T(t))</math>, <math>dP(T(t))/dt</math>, <math>M(T(t))</math>, <math>dM(T(t))/dt</math></li></ul> <p>extended features for High Sensitivity Isothermal Heat Flow Calorimetry (HFC): Ability to calculate the thermokinetics from long term isothermal HFC data for very precise lifetime prediction on the first percent of degradation (quality control)</p>	10'000.-	x1	10'000.-

(Upgrade: includes one (1) year subscription for free upgrade)

Determination of the heat accumulation and temperature of the runaway reactions of energetic materials under adiabatic and non-adiabatic conditions.

*The Thermal Safety version requires the Thermal Aging version. It contains the same options as in Thermal Aging version with several additional thermal safety features.*

► **Determination of the thermal stability of energetic materials under adiabatic conditions:**

- determination of the Time to Maximum Rate under adiabatic conditions (TMRad) for any chosen starting temperature, for simulation of e.g. BATCH reactors in case of cooling failure, storage, transport, scale-up
- 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 self heat rate curves  $dT/dt$ ,  $dQ/dt$ ,  $d\alpha/dt$  and  $dP/dt$  (possible with a C-80 for pressure/gas generation quantification for subsequent vent sizing calculations), determination of the temperature corresponding to ARC detection limit such as 0.02 K/min, ...

► **Determination of the heat accumulation and temperature of the runaway reactions under non-adiabatic conditions:**

- determination of the effect of properties of the chemicals and containers on the reaction progress and heat accumulation conditions for the simulations of runaway reactions. This analysis combining Finite Element Analysis and thermokinetics is applied for the determination of the critical design parameters i.e. construction of a thermal safety diagram under non-adiabatic conditions (TMR = f(r,  $T_{in}$ ,  $\lambda$ ,  $\rho$ , cp,  $T_{out}$ )) = runaway time as a function of any process parameters such as
  - radius 'r' of e.g. containers
  - hot discharge temperature ' $T_{in}$ '
  - thickness 'd' of the insulation
  - chemical properties: thermal conductivity ' $\lambda$ ', density ' $\rho$ ', specific heat 'cp'
- surrounding temperature ' $T_{out}$ ' for safe storage or transport conditions. Possibility to predict the reaction rate and heat accumulation conditions for any surrounding temperature profiles such as isothermal, stepwise, modulated, shock, NATO Norm STANAG 2895, customized T-profiles and additionally for T-profiles reflecting different climates.
- automatic procedures for the 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
- fire exposition considerations: heat transfer coefficient considerations (radiation and convection) according to European Norm EN1991-1-2/2002

numerical algorithm based on finite element, finite volume and difference method with non-uniform adaptive spatial and time mesh. Applications of explicit and implicit methods: this approach leads to a differencing scheme that is second order accurate in both space and time and stable for large time steps. It ensures high precision and decreases by orders of magnitudes the calculation time

- presentation of the temperature and conversions distribution on 3-D graph with
  - temperature and concentration distribution on the color-gradient graph
  - animated view of variation of temperature distribution in time and in space color-gradient graphs

User friendly help with live videos and graph saving in \*.gif formats with automatic exportation in MSWord for easy reporting

3	<b>AKTS-Training class</b>	1'200.-	x2	2'400.-
	Two days (2)			
	<b>Expenses to cover accommodations and travel fees</b>	0.-		0.-

**Summary of the training class:**

1. Baseline determination and kinetics
  - 1.1 Definitions
  - 1.2 Kinetics overview - isoconversional methods: Friedman, Ozawa, ASTM A698
  - 1.3 Baseline determination and initialization
  - 1.4 AKTS' methods: Computation of kinetics and baseline optimization
  - 1.5 Prediction of the reaction progress under any temperature modes
    - isothermal, non-isothermal - stepwise - modulated temperature or periodic temperature variations - rapid temperature increase (temperature shock) - real atmospheric temperature profiles (climates) - STANAG 2895
    - customized T-profiles
  - 1.6 Confidence interval of the predictions
  - 1.7 Exercises: AKTS-Thermokinetics Software – Thermal Aging Version
2. Thermal risk
  - 2.1 Kinetics and adiabatic conditions (Time To Maximum Rate under adiabatic conditions – TMRad, ARC  $\phi=1$  and  $\phi>1$ , heat rate curves, thermal stability diagram under adiabatic conditions)
  - 2.2 Exercises: AKTS-Thermokinetics - Thermal Safety Version
  - 2.3 Kinetics and non-adiabatic conditions (Finite Element Methods)
  - 2.4 Heat accumulation, thermal runaway
  - 2.5 Exercises : AKTS-Thermokinetics - Thermal Safety Version
3. Case study and risk analysis
  - 3.1 Thermal runaway scenario - 3.2 Gravity - 3.3 Probability
  - 3.4 Thermal stability diagram under non-adiabatic conditions: Determination of the critical parameters : radius, insulation, surrounding temperature, hot discharge temperature, SADT, fire radiation & convection according to EN1991-1-2/2002
  - 3.5 Thermal security, storage and transport
  - 3.6 Exercises : AKTS-Thermokinetics - Thermal Safety Version

<b>Subtotal</b>	EUR	22'400.-
<b>VAT(*)</b>		
<b>Total amount due</b>	EUR	22'400.-

(\* Switzerland: VAT 7.6%.

Rest of the world: taxes, value-added or any other governmental charges imposed are at the charge of the user).

### AKTS-Training class information

AKTS will give two days AKTS-Training class at customer place. The two days AKTS-Training class usually starts at 8h00-8h30 (depending on the wishes of the participants) and finishes at 18h00. The AKTS-Training class consists in one hour presentation of AKTS-Thermokinetics software followed by about 15-30 kinetic analyses of 4-6 thermoanalytical curves (DSC, TG...) starting from simple curves to complex multistage overlapped reactions (10-15 kinetic and thermal safety analyses the first day and 15 analyses during the second day). The intensive training provides a balance between theory and practical applications through the exercises. For each exercise the participants have to construct the baseline on the DSC signals and after baseline optimization and determination of the kinetics the following types of questions have to be answered:

- What is the activation energy of the reaction as a function of the reaction progress?
  - At which temperature there is a conversion of 50% after 2 days?
  - What is the reaction progress at 25 °C and at 25 °C±10 °C after 1 year?
  - At each temperature, what is the Time To Maximum Rate under adiabatic conditions TMRad?
- => Construction of a safety diagram: runaway time as a function of process temperature under adiabatic conditions (TMRad = f(T)).
- Based on the safety diagram TMRad=f(T): what temperature leads to a TMRad of 24h? of 8h?
  - What is the critical radius of a container for a hot discharge temperature corresponding to a TMRad of 24h?
  - What is 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?

For the AKTS-Training, a class room with one computer per participant is requested (or the participants can use their own laptops). This is important because each participant will have to perform individually all kinetic analyses and exercises during that intensive day. Problem definition, baseline constructions, kinetics and results visualisation and interpretation for the prediction of the thermal stability and runaway are covered in details.

Possible AKTS-Training Languages: English, German, French and Chinese.

## Pricing:

Each AKTS-Training class at new user worldwide locations is charged 1'200 EUR/day.

Expenses for accommodations and travel fees at worldwide locations:

Switzerland : 0 CHF

Germany, France, Italy, Austria : 500 EUR

Rest of Europe: 800 EUR

USA : 1'500 EUR

Asia and rest of the world : up to 2'200 EUR

## Overview of AKTS-Thermokinetics Version 3

### - Thermal Aging

- **Overview:**

<http://www.akts.com/thermal-aging-overview.html>

### - Thermal Safety

- **Overview:**

<http://www.akts.com/thermal-safety-overview.html>

## Webinar of AKTS-Thermokinetics Version 3

<http://www.akts.com/akts-thermokinetics-tga-dsc-dta-tma-ftir-ms/akts-thermokinetics-help-e-learning.html>

*(Note: it might take up to 30 sec to start the video depending of the load on the system)*

Direct links:

Video / webinar (45 min):

<http://www.akts.com/video-webinar-e-learning.html>

Pdf (22MB) / slides (100):

<http://www.akts.com/video-webinar-e-learning-pdf.html>

## Example of Studies / Papers

- Thermal Aging Studies / Papers

<http://www.akts.com/akts-thermokinetics-tga-dsc-dta-tma-ftir-ms/akts-thermokinetics-technical-comments.html>

- Thermal Safety Studies / Papers

<http://www.akts.com/time-to-maximum-rate-adiabatic/runaway-reactions-akts-thermal-safety-software-technical-comments.html>

## Upgrade/maintenance

- Includes one **(1) year** subscription for free upgrades

## Deliverables

AKTS-Thermokinetics Software version 3 is available for immediate download and it is also sent by FedEx as soon as Purchase Order received. Electronic keys for the activation of AKTS-Thermokinetics Software are delivered by email or by direct online activation through the internet.

- Thermokinetics, Thermal aging, Thermal safety (TMR<sub>ad</sub>):

<http://www.akts.com/akts-thermokinetics-how-to-upgrade.html>

- Thermal safety (SADT):

<http://www.akts.com/thermal-safety-how-to-upgrade.html>

## VIEWER versions

Besides the 'Licensed' version, AKTS delivers to your institute **an unlimited number** of 'VIEWER' versions. These VIEWER versions **are free of charge** and can be installed on several computers. They can be downloaded at any time from the following links:

<http://www.akts.com/thermal-aging-overview.html>

or

<http://www.akts.com/thermal-safety-overview.html>

The sole difference with the 'Licensed' version is that the 'VIEWER' versions cannot elaborate the new measured data. However, the VIEWER versions can open the 'analysis files' previously created with the 'Licensed' version. Additional copies of the 'VIEWER' versions can be made without the written permission of AKTS. These viewer versions are very highly appreciated for advanced and efficient reporting of data analysis.

Thank you for your interest in AKTS Software.

AKTS AG - Switzerland

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## **SUPPORT AND MAINTENANCE INFORMATION**

### **Thermal Aging and Thermal Safety Versions**

#### **Introduction**

Thank you for purchasing a support and maintenance contract for AKTS-Thermokinetics Software denoted hereafter « AKTS-Software ». At AKTS AG, we know that time is critical when it comes to your research, development and production. That is why AKTS AG' Support is organized to respond quickly and accurately to meet your needs. Our support engineers help resolve your difficulties you may have with our products and suggest efficient ways of achieving your development objectives. In addition, we offer optional consulting services for those needing special tools or libraries for « AKTS-Software » and your specific operating system/environment. Each AKTS AG Support and Maintenance Contract Offers:

- Support response in two business days or less.
- Access to the web site for maintenance releases and patches, and unlimited email support.
- Free upgrades to the latest version of AKTS-Software when released.
- Each support and maintenance contract is limited to support up to 2 engineers on one project.

This guide introduces you to the support services available from AKTS AG and instructions on how to use them. Specifically, it tells you how to access these services, and how to make the most effective use of them. Purchasing AKTS AG Support is assurance in having access to the AKTS-Software support engineers when you need them the most – meeting a critical deadline, needing help through a tough problem, finding work-arounds or fixing tool bugs.

#### **How to Request Support**

Internet email and telephone help desk are the two ways to contact AKTS AG.

- info\_contact@akts.com
- phone : +41 848 800 221

If AKTS AG received a question by email, an engineer will follow-up with a telephone call or email (usually within one business day or less), depending on workload and nature of the question. The customer will be notified as to an estimated time for problem resolution.

#### **Escalation of Problem Reporting**

- a. Normally most questions are resolved through user assistance and initial collaboration.
- b. If the problem cannot be resolved during the initial contact, it is escalated to an SPR (Software Problem Report). An SPR is opened and referred to a subject matter expert who is specifically equipped to deal with support issues in his product area. He will continue to work the SPR to resolution, or until a software problem is identified.
- c. If not resolved at the SPR level (i.e., a defect is identified), the support engineer issues a Software Change Request (SCR).

AKTS AG engineering evaluates the nature of the software issue, to determine the optimum nature of resolution for the SPR. Depending on severity, level of urgency, and schedule, AKTS AG engineering may recommend one or more of the following options:

- **Workaround.** A specific methodology for mitigating the impact of the software problem, which may be implemented on an expedient basis to allow customer development to proceed.

- **Version Patch or Build.** If the software problem can be isolated / diagnosed to a small region of code that is easily modifiable, AKTS AG may elect to provide the customer with a custom rebuild of the effected software component(s). This also provides an expedient path for resumption of customer development. Normally these SCRs will be fed into the normal software engineering upgrade cycle, such that fixes are automatically incorporated into future maintenance releases.
- **Custom/ECP.** In some cases, software enhancements are proposed by customer. If the proposed software enhancements can be easily implemented, these new features will be fed into the normal software engineering upgrade cycle and incorporated into future maintenance releases. However new features that will require major software development effort to implement (typically this implies development scope requiring many source lines of code). In such cases AKTS AG will develop an Engineering Change Proposal (ECP) outlining the cost, resources, and schedule requirements for implementing the new features. This ECP will serve as the basis of negotiations between AKTS AG and our development partners for cost (and benefit) sharing of the proposed software enhancements.

### Summary of Escalation Levels

- a. Internet email and telephone help desk
- b. Software Problem Report (SPR)
- c. Software Change Request (SCR)
  - Workaround
  - Patch/Build
- d. Custom Development via Engineering Change Proposal (ECP)

### Web Site Support Features

AKTS AG has a web site with support pages that gives you access to the following features:

- On-Line Documentation
- Knowledge Base
- Maintenance Releases
- Downloads/Upgrades

By registering a AKTS AG product, the customer receives access to all of the web site support features for free. Purchasing support gives the customer the added benefits of help desk support and problem resolution. The AKTS AG web site is continually evolving. Information is update, and new features are added regularly. We encourage you to visit the site frequently to see new features.

### Help Us Help You Making an Inquiry

Each customer should designate per license one person as technical contact per AKTS AG terms and conditions for Support and Maintenance. When a question or problem comes up, your technical contact should be the person directing the inquiry to Support. AKTS AG support maintains a list of customer technical contacts. We understand that personnel may change. Please keep us informed of your current technical contact by contacting AKTS AG.

### How to Get Answers, Fast!

When you call, we want to help you use time efficiently. If you have the following information at your fingertips, it will help us to help you more quickly:

- AKTS AG Product
- AKTS AG Version
- Host Platform
- Upgrade question
- Thermokinetic question
- Thermal Safety question

You can help us resolve your question more quickly if you're also prepared with a clear description of the problem and any associated problems you encountered in a test case (some screen captures or a quick approach to reproducing the problem may be helpful).

### Your Feedback

AKTS AG is committed to responding to customers quickly and accurately. We welcome your comments regarding our support. Your feedback will help us maintain the highest level of service.

## Upgrade instructions for AKTS-Software

Thermokinetics, Thermal aging, Thermal safety (TMR<sub>ad</sub>):  
<http://www.akts.com/akts-thermokinetics-how-to-upgrade.html>  
Thermal safety (SADT):  
<http://www.akts.com/thermal-safety-how-to-upgrade.html>

## Terms and Conditions

### Introduction

These terms and conditions apply to each Support and Maintenance Contract. Your purchase of a Support and Maintenance Contract is an acceptance by you of these terms and conditions.

### Support

This Agreement entitles you to obtain technical support services ("Support") from AKTS AG. Support means answers to questions, guidance, and assistance as determined by AKTS AG. Support excludes configuration of hardware, software, and networking equipment and software that are not products of AKTS AG. It excludes general computer system maintenance and consulting services that are not in direct relation with AKTS-Software. You are responsible for performing operations on your computer system, and AKTS AG shall have no responsibility to perform operations on your computer system. You agree to provide AKTS AG all information reasonably requested by AKTS AG to enable AKTS AG to provide Support. Such information may include, but not be limited to, the type of hardware you are using, a description of the problem for which you seek Support, and additional software you are using that falls outside the subject matter scope of coverage. You understand and agree that the completeness and accuracy of the information you provide to AKTS AG pursuant to this section may affect AKTS AG's ability to provide Support.

### Subject Matter Scope of Coverage

AKTS AG will provide Support for the official customer site where AKTS-Software product has been licensed and installed. AKTS AG will provide Support for AKTS-Software only and for other customer sites where AKTS-Software product has been licensed. You understand and agree that AKTS-Software may not function with certain hardware systems and components. Such hardware is unsupported hardware. AKTS AG shall have no obligation to provide Support for any system that is or that includes unsupported hardware.

### Availability of Coverage

You are entitled to seek Support from 9:00 AM till 12:00 AM and from 1:00 PM till 5:00 PM Central Europe Time Monday through Friday, excluding holidays, throughout the term of this agreement. Holidays include, but may not be limited to, the Swiss holidays. In the event that one of these holidays falls on a Saturday, the preceding Friday shall be a holiday. In the event that one of the holidays falls on Sunday, the following Monday shall be a holiday.

### Who May Seek Support

Only the official sites where AKTS-Software has been licensed may seek Support from AKTS AG. You are responsible for all persons who seek Support pursuant to this agreement. AKTS AG shall have no responsibility for any unauthorized use of Support.

### Response Times

AKTS AG shall respond to requests for Support within two business days of receipt of your request for Support. A response to a request for Support may consist of a receipt of and acknowledgment by AKTS AG of your request for Support. You acknowledge and understand that no software is perfect or error free, and that despite its commercially reasonable efforts, AKTS AG may be unable to provide answers to or resolve some or all requests for Support. AKTS AG makes no promises, guarantees or assurances of any kind that it will be able to provide the support services you seek. We do promise to do our best to satisfy each customer, whether it be complete software fixes, upgrades or workarounds to a problem.

### Payment

Any and all payments made by you pursuant to this agreement shall be nonrefundable. There shall be no refunds or credits for any unused Support or other unused services upon the termination of this agreement for any reason or at any other time. In the event that you fail to pay AKTS AG pursuant to this agreement, AKTS AG's obligations to provide Support shall be suspended until AKTS AG receives full payment for all fees, including late fees and interest, due to AKTS AG.

### **Duration and Pricing** (Please check the desired option)

Purchasing of AKTS-Software licenses includes **one (1) year** subscription for free support and upgrades from the time of the license activation. Then (optional):

One (1) additional year **SUPPORT AND MAINTENANCE AND UPGRADE CONTRACT:**  
10% of license price = 2'000 EUR /license /year

Three (3) additional years **SUPPORT AND MAINTENANCE AND UPGRADE CONTRACT:**  
8.5 % of license price = 1'700 EUR /license /year

Five (5) additional years **SUPPORT AND MAINTENANCE AND UPGRADE CONTRACT:**  
7 % of license price = 1'400 EUR /license /year

(All given prices are valid until December 31<sup>st</sup> 2010.)

### **Termination**

Either party may terminate this agreement at any time. Termination of this agreement does not relieve your payment obligation for Support provided to you by AKTS AG.

### **No Transfer**

Any reuse, transfer, assignment, or distribution of Support without the prior written permission of AKTS AG is prohibited. Any attempt to transfer, assign, or redistribute Support in violation of this section shall be a violation of this agreement and shall immediately terminate this agreement and all your rights under it.

### **No Warranty**

Support, other services, information, and software provided to you by AKTS AG are provided "as is" without warranty of any kind, express, or implied, including, but not limited to, the implied warranties of merchantability, fitness for a particular purpose, and non-infringement.

### **Limitation on Liability**

Neither you nor AKTS AG shall be in breach of this agreement due to any failure of performance that arises out of causes beyond its reasonable control. AKTS AG shall not be liable to you or to any third party for any indirect, special, incidental, or consequential damages in connection with or arising out of this agreement, including, but not limited to, lost profits or lost data in connection with this agreement, even if AKTS AG had been advised of the possibility of such damages. AKTS AG will not be liable to you on account of errors, omissions, delays or losses.

### **General**

This contract is governed by the laws of Switzerland. Venue is Sion (VS), Switzerland. This contract gives you specific legal rights; you may have others which vary from state to state and from country to country. AKTS reserves all rights not specifically granted by this contract. Any dispute arising out of this contract shall be adjudicated solely in the applicable federal or state courts within Switzerland.

This contract, including all schedules, constitutes the entire understanding of the parties. This contract supersedes and terminates all prior representations, warranties, and agreements, written or oral, regarding the subject matter of this agreement. Any modification to this contract must be in writing signed by both parties.

In consideration of this contract, you are responsible for paying the license fees of AKTS-Thermokinetics Software. The amount is payable without any deduction for taxes, assessments, fees, or charges of any kind.

### **CONTACT**

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