

Thermal Safety Series - Advanced Reaction Kinetics Simulation

TSS-ARKS

Software

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Email: office@cisp.spb.ru; Web: <http://www.cisp.spb.ru>



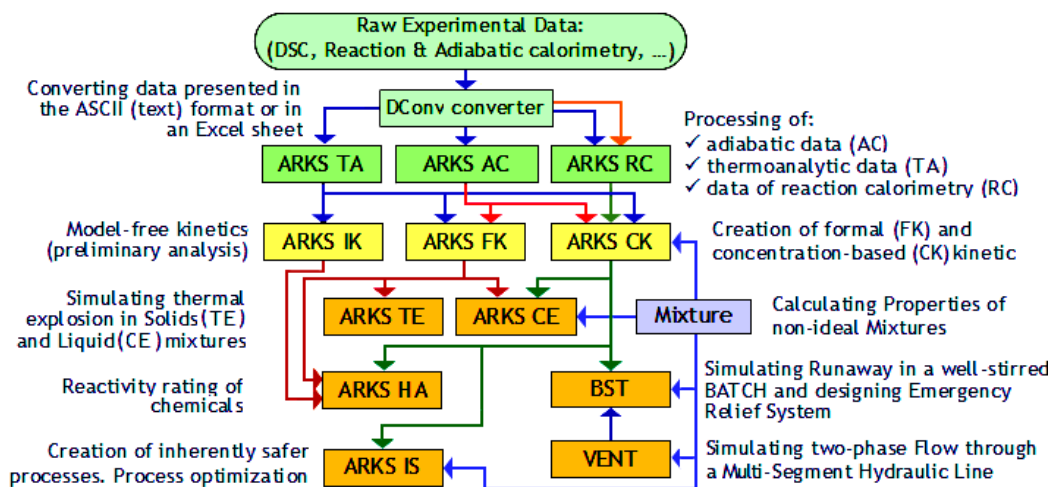
Thermal Safety Series - Advanced Reaction Kinetic Simulation (TSS-ARKS) Software

the analog-free methodology and software for reaction hazard assessment of Chemical Processes and Products.

At CISP, we strongly believe that the future of the process' and products' safety science relies more on digitally - based methods. To achieve this transformation, we associate methods of calorimetric experiments, kinetics evaluation and process simulation with software development to help you through all phases of your projects.

To support your research work CISP devises a synergistic concept which includes methods, TSS-ARKS software and consulting services. CISP offers:

- The state-of-the-art methods for interpretation and analysis of data from various calorimetric techniques;
- Powerful methods for creation of kinetic reaction models of various types;
- The state-of-the-art simulation-based methodology for predicting and preventing runaway accidents involving chemical products and processes;
- All the methods are supported by user-friendly TSS-ARKS software allowing a researcher to concentrate on the problem at hand rather than on challenges related to ways of solving problems;
- TSS-ARKS components are interlinked to each other providing a unified analog-free system;
- Each TSS-ARKS component has a unique set of features that distinguishes it from other commercial offerings. TSS-ARKS components can be used successfully as standalone programs.



General features of the Software

- System of interlinked components based on sophisticated methodology
- Application of state-of-the-art math methods
- Merger of math methods and experience of a researcher into unified strategy
- Management of multiple projects
- Link to Physical Property Data Bases
- Flexible graphics
- Common data bases of kinetic models
- Common elements of project-oriented User's interface
- Manipulated accuracy control
- MS Word report generation
- Interactive help system
- [Video lessons for every application to help in mastering them](#)
- Complete set of user manuals
- Minimum hardware requirements: Pentium V, multi-core, Windows 7, 8, 10 MS Word and Excel 2003 - 2013 installed

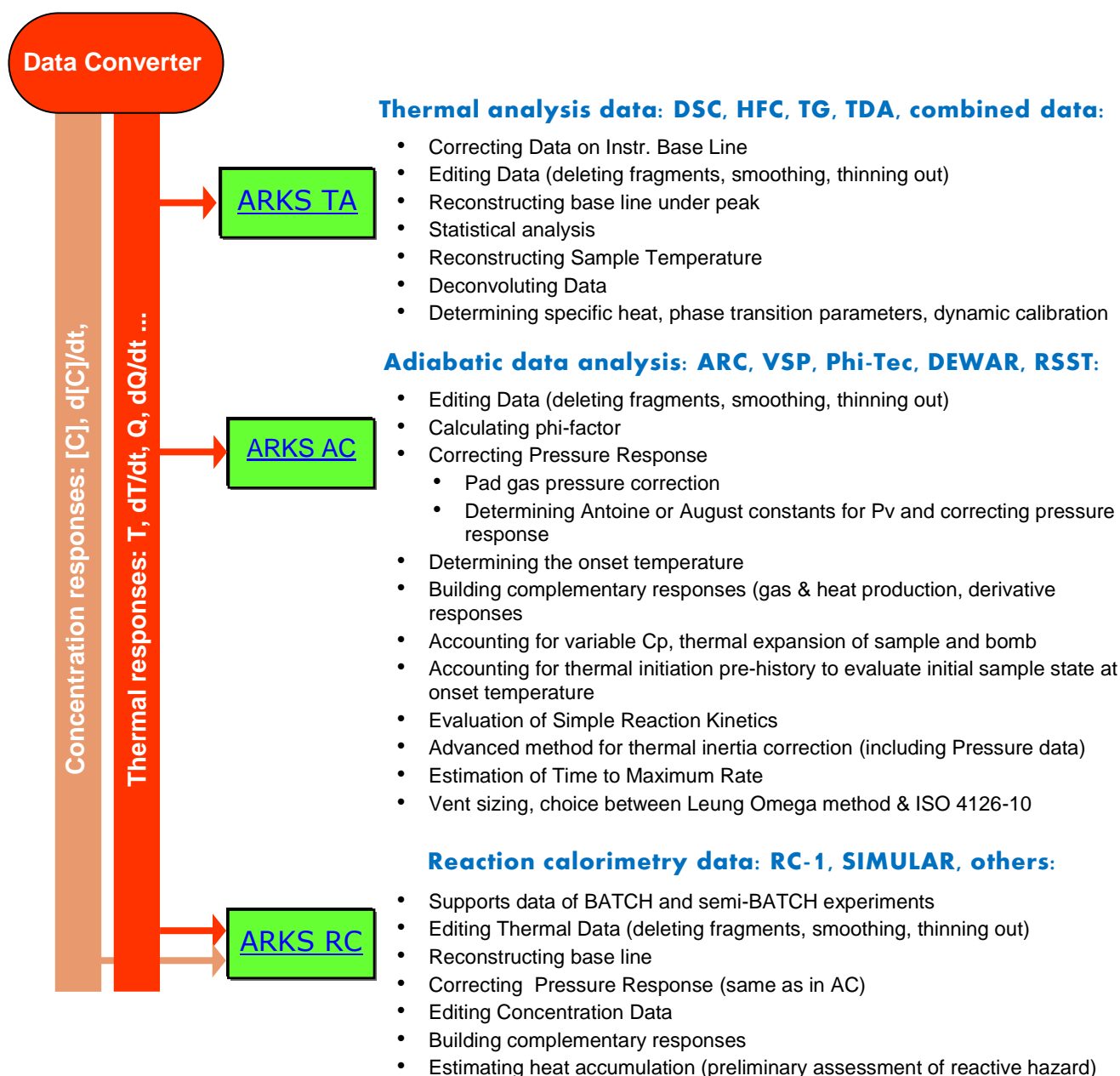
TSS-ARKS – to whom it is addressed

- R&D Centers of Chemical and Pharmaceutical Companies;
- R&D Centers of Manufacturers and Users of energetic materials;
- R&D Centers of Manufacturers and Users of rechargeable batteries
- Physical-chemical laboratories
- R&D Centers involved in hazard assessment of dangerous goods (UN TDG, IMO, etc.), and in classification of chemicals (UN GHS, CLP, etc.);
- Consulting Firms dealing with Chemical Processes;
- Chemical Engineering Departments of Universities

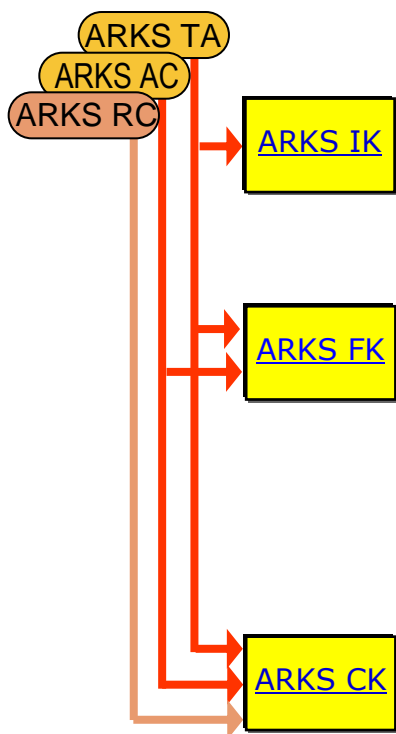
TSS-ARKS - successor of the well-known TSS series

TSS-ARKS inherits all the best qualities of TSS. TSS-ARKS applications have more up-to-date interface, improved algorithms, new useful options, completely revised helps and manuals and more.

Applications for processing of experimental data



Applications for kinetics evaluation



Isoconversional kinetics: Fast preliminary kinetic analysis:

- Revealing reaction complexity
- Generating initial guess on activation energies
- Modeling of reaction course within temperature range covered by experiments
- Rough estimates of hazard indicators (adiabatic TMR, thermal stability)

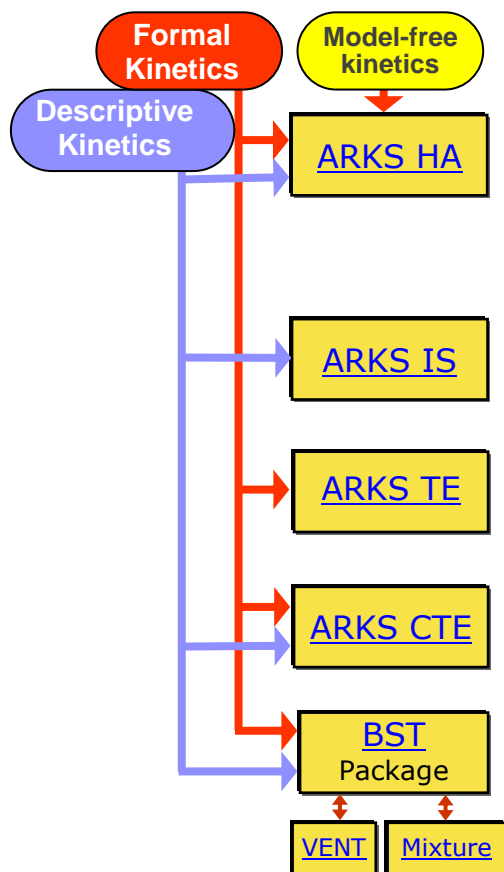
Formal conversion-based models:

- Simultaneous use of multi-response data of different experiment's types
- Evaluation of complex formal models by using non-linear optimization
- A model may include several independent, parallel and consecutive stages
 - Branched pathways
 - Reversible stages
 - Pressure-dependent stage rates
 - Model with melting
- Easy method for creation of a complex model without programming
- Simulation of well-stirred BATCH under variety of thermal modes
- Calculation of hazard indicators (adiabatic TMR, thermal stability)

Descriptive concentration-based models:

- Simultaneous use of multi-response data of different experiment's types
- Automatic creation of multi-stage models from stoichiometric reaction scheme, a stage rate obeys generalized law of mass action (Optional) liquid+vapor reactions, reactions on tank surface
- Evaluation of complex models by using non-linear optimization
- Simulation of well-stirred BATCH, semi-BATCH, CSTR and Plug Flow reactors under variety of thermal modes
- Calculation of hazard indicators (adiabatic TMR, thermal stability)

Applications for Reaction Hazard Assessment (coming soon)



Assessing Hazards:

- Automatic determination of NFPA reactivity number – standard and advanced methods
- Automatic determination of adiabatic TMR, ADT24 & TER
- Automatic estimate of Thermal Stability (TCL) and thermal aging, accounting for seasonal variations of temperature
- Automatic determination of SADT for liquids in accord with TDG and GHS requirements
- Vent sizing, Leung Omega method or ISO 4126-10 (coming soon)

Design of Inherently Safer Processes:

- Providing safety of normal operational mode
- Providing maximal possible safety in case of accident
- Analyzing sensitivity of thermal mode to controls deviations

Assessing Reaction Hazard of Solid Products:

- Automatic determination of SADT (UN H1 test)
- Automatic determination of critical temperature
- Runaway simulation for variety of geometries

Assessing Reaction Hazard of Liquid Products:

- Automatic determination of SADT (UN H1 test)
- Automatic determination of critical temperature
- Runaway simulation for variety of geometries

Designing ERS:

- Simulation of runaway in a BATCH reactors
- Calculation of 2-phase flow along multi-section pipeline
- Sizing safety devices

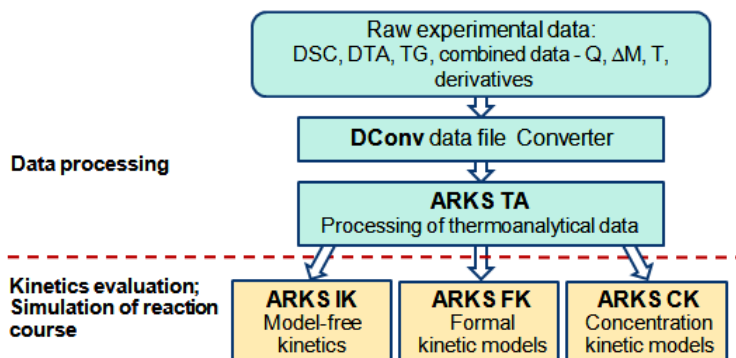
Ready Solutions

The TSS-ARKS software includes more than 12 applications. In many cases there is no need to use all of them. Moreover, though the primary aim of TSS-ARKS is to help in reaction hazard assessment its components can be successfully used in various researches that are not related with hazards. We can offer several sub-sets adjusted for specific areas of application..

You won't find here the exhaustive specifications of the programs that compose the sub-sets proposed. We mentioned only some features that are relevant to the area of application. Request TSS-ARKS specifications for more detailed description.

The sub-set for thermal analysis

This subset is specified for physical-chemical laboratories that primarily apply methods of thermal analysis.



It consists of ARKS TA, FK and/or CK and/or IK.

ARKS TA is the powerful data processing program capable of handling data from various calorimetric instruments (DSC, heat flow calorimetry, DTA), TG data, and data from combined methods (DSC+TG, DTA+TG). It not only allows comprehensive processing of original experimental data but also supports determination of physical properties of a substance such as specific heat capacity, parameters of phase transition, thermal conductivity of liquids.

The auxiliary DConv data converter program allows simple method for data conversion so that ARKS TA can be used in combination with any thermal analytical instrument.

The line of programs **ARKS FK/CK/IK** allows evaluation of reaction kinetics of various kinds. The choice depends on the kind of investigations carried out in the laboratory. Typical choice for a thermo-analyst would be either ForK or IsoKin but we recommend considering them as a pair of mutually complementary programs.

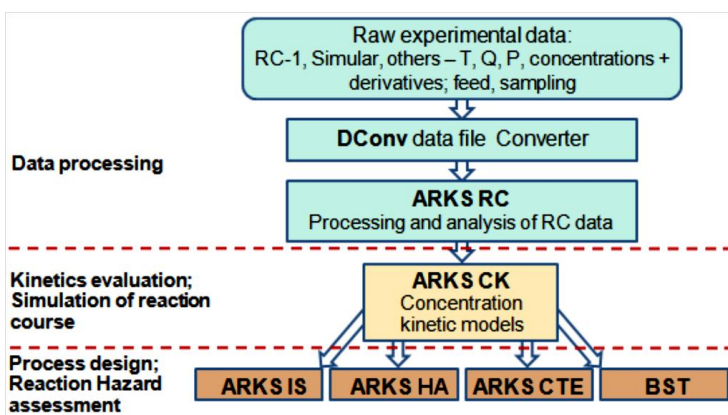
All the programs have powerful modules for simulation of reaction course under various conditions; hence they can be successfully used for solving various practical problems from analysis of thermal stability to estimation of thermal mode of a reactor.

ARKS IK supports creation of the so-called model-free kinetics. It is the convenient tool for easy and fast preliminary analysis of data.

ARKS FK is designed for creation of conversion-based complex multi-stage formal models.

ARKS CK allows creation of more habitual concentration-based models of complex reactions.

The subset for reaction calorimetry



This subset is intended for a chemical engineering laboratory which investigates chemical reactions by applying reaction calorimetry or lab-scale reactors. It consists of ARKS RC, CK, IS and/or ARKS RR and/or CE and/or BST Package.

ARKS RC provides processing of data that include heat generation, pressure and concentration responses. Data can be generated by experiments run in BATCH or semi-BATCH mode with multi-component reacting mixtures. The auxiliary DConv data converter program allows simple method for data conversion. ARKS RC can be used in combination with any available reaction calorimeter. The latest version of the program supports estimation of heat accumulation in a reactor thus allowing preliminary assessment of reactive hazard

ARKS CK allows creation of complex multi-stage concentration-based reaction models. The bunch of the state-of-the-art math methods for numerical integration of non-linear reaction models and non-linear optimization in conjunction with calculation of variable physical-chemical properties of mixtures makes this program the analog-free tool for kinetic analysis.

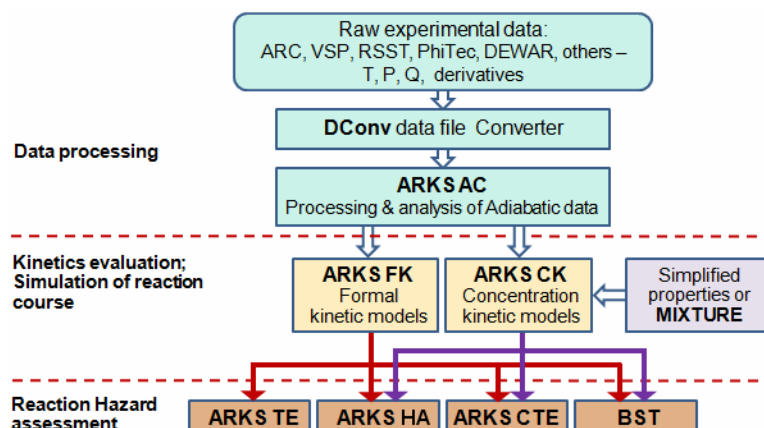
The line of programs **ARKS IS/HA/CTE/BST** allows solving various practical problems. The choice depends on the kind of investigations carried out in the laboratory.

ARKS IS can help in designing a process. It allows process optimization, includes the unique method for designing an inherently safer process, and has the analog-free module for stability analysis of a process mode. ARKS IS can be recommended to anyone involved in chemical engineering.

The subset for adiabatic calorimetry

Adiabatic calorimetry of various kinds (ARC, VSP, DEWAR, etc.) is the method that had been specifically designed for study of reaction hazards. Therefore this subset is adjusted for a laboratory which primary interest is in reaction hazard assessment. The subset includes ARKS AC, FK and/or CK, and the pack consisting of ARKS TA, HA, CTE and BST.

ARKS AC is the unique data processing program capable of handling temperature and pressure data from various adiabatic instruments (ARC, VSP, Phi-Tec I and II, DEWAR and others).



The auxiliary DConv data converter program allows simple method for data conversion so that ARKS AC can be used in combination with any type of adiabatic calorimeter. The program package offers the unique set of advanced data analysis methods such as kinetics evaluation, analog-free advanced method for thermal inertia correction, adiabatic TMR calculation and vent sizing.

ARKS FK (ForK) and/or CK (DesK) are used for kinetics evaluation. The choice depends on the laboratory profile. If the primary interest is in hazard assessment of reactive chemicals (especially solids) then ARKS FK would be the right choice. If the laboratory is involved in process safety studies then we would recommend considering ARKS CK as a candidate. The pair ARKS FK+CK covers a wide range of problems and therefore provides maximal flexibility.

ARKS IK supports creation of the so-called model-free kinetics. It is the convenient tool for easy and fast preliminary analysis of data. **Evaluation of model-free kinetics based on adiabatic data is the unique feature of the program.**

ARKS FK is designed for creation of conversion-based complex multi-stage formal models.

ARKS CK allows creation of more habitual concentration-based models of complex reactions.

The last group of programs serves for assessment of reaction hazards.

ARKS TE and **CTE** are for simulation of thermal explosions in solids and liquids.

ARKS HA provides easy and fast determination of hazard indicators of chemicals.

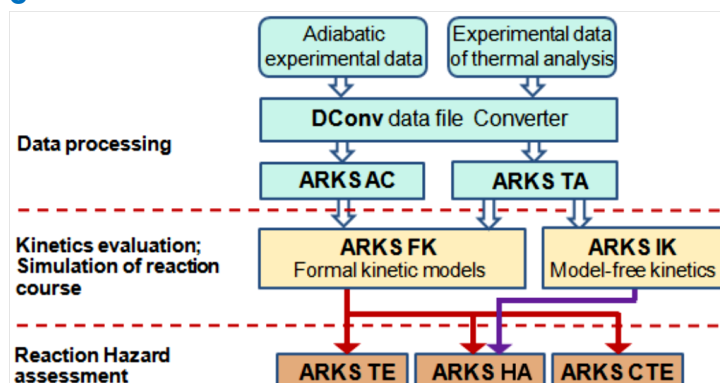
BST package is intended for design of emergency relief systems.

The appropriate composition of the last group also depends on the laboratory profile. For those who mostly involved in determination of hazardous characteristics of reactive chemicals the triplet ARKS RR- TE - CE can be recommended whereas for specialists in ERS design BST would be of primary interest.

The subset for hazard assessment of energetic materials

Nowadays considerable efforts are concentrated on hazard assessment of energetic materials. The final aim of such investigations is the proper choice of safe conditions of use, storage and transportation of these substances. Typical experimental methods in this field include thermal analysis and adiabatic calorimetry.

Taking into account specific features of methods applied and practical tasks to be solved, we can propose the following subset that includes ARKS AC, TA, FK and IK, and ARKS RR, TE and CE.



ARKS TA and **AC** support all necessary types of data processing for data of thermal analysis and adiabatic calorimetry. The auxiliary DConv data converter program allows simple method for data conversion so that ARKS TA and AC can be used in combination with any thermal analytical and adiabatic instrument respectively.

ARKS IK is the convenient tool for easy and fast preliminary analysis of data by applying model-free kinetics. Results of this analysis are helpful for creation of formal kinetic models that are evaluated by using **ARKS FK**. These models are the basis for assessing hazard by applying the last group of programs.

ARKS FK is designed for creation of conversion-based complex multi-stage formal models.

ARKS HA provides easy and fast determination of hazard indicators of chemicals whereas

ARKS TE and **CTE** provide in-depth analysis of thermal explosion hazards of solid and liquid chemicals as well as

thermal modes of BATSH reactors.

ARKS TE simulates thermal modes of the objects with solid chemicals on the basis of thermal conductivity equation coupled with kinetics and takes into account temperature and conversion profiles that appear in an object. Thanks to new features of the latest version of ARKS-TE it allows analysis of much wider range of cases including thermal modes of industrial reactors.

ARKS CTE is a CFD code which allows simulation of the vessels with liquid reactant and is based on numerical integration of the Navier–Stokes model coupled with kinetics. Simulation takes into account heat transfer due to conductivity and convection and convective mass transfer.

CISP operates worldwide in partnership with:

- Thermal Hazard Technology (THT), UK;
- H.E.L. Group Ltd., UK;
- Sumika Technical Information Service, Inc., Japan;
- MYJA Technology Co., Ltd, China;
- Chemryt Informatics Pvt Ltd., India;

CISP Newsletters available on <http://www.cisp.spb.ru/newsletters>

1. Kinetics-based simulation – how can this approach help when assessing reaction hazard?

The first newsletter from the series aimed at better acquaintance with the features of the simulation-based approach to reaction hazard assessment and CISP TSS-ARKS software.

2. Kinetics-based simulation – how can this approach help when assessing reaction hazard? Examples, part 1

In many cases even routine problems require application of kinetics-based simulation for getting correct results. Part 1 demonstrates several examples of this kind:

- Correction of adiabatic data on thermal inertia;
- Calculation of time to maximum rate (TMR) and estimation of thermal stability of a compound;
- Determination of reactivity rating number (RRN).

3. Kinetics-based simulation – When can it help while assessing reaction hazard? Examples, part 2 - Applying the approach for simulation of thermal explosions.

Firstly the overview of the well-known simplified analytical theories is given, their merits and limitations are discussed. Then the more general simulation-based method is specified and illustrated by some examples

4. Kinetics-based simulation – When can it help while assessing reaction hazard? Examples, part 3.

It continues discussion of other examples - design of the Emergency Relief System (runaway simulation and vent sizing), and design of an inherently safer process.

The first example demonstrates how simulation results have been validated by the pilot-plant experiment.

The second example shows, how heat exchange in a jacketed semi-batch reactor is taken into account.

5. Applying the Kinetics-based simulation approach for determination of the SADT. Examples, part 4.

This issue demonstrates application of DSC for kinetic study and the use of DSC-based kinetics for determination of the Self-Accelerating Decomposition Temperature (SADT) by numerical simulation. The example is based on real data regarding the decomposition of 50% solution of hydroxylamine in water.

6. Kinetics-based simulation approach. Identification of Kinetic Models for the Assessment of Reaction Hazards.

This newsletter gives the overview of the state-of-the-art method of kinetics evaluation applied in TSS-ARKS. It allows creation of complex multi-stage kinetic models capable of describing reactions occurring in chemical products and in chemical reactors (synthesis reactions).

7. Kinetics-based simulation approach. Model-free versus Model-based kinetics: Pros and Cons.

This issue gives the objective comparison of two alternative kinetics evaluation methods - model free versus model-based one. Merits and limitations of the model-free kinetics are discussed. It is shown that both the methods are mutually complementary rather than antagonistic: model-free method is very useful for fast preliminary evaluation that must be followed by more in-depth model-based kinetic analysis.

8. Evaluation of reactive hazard of Li-ion battery

The newsletter gives the example of applying the kinetics-based simulation approach for hazard assessment of Li-ion battery - namely kinetics evaluation from adiabatic data.

9. Kinetics-based simulation approach. Advanced analysis of adiabatic data by applying ADaExpert

This issue demonstrates the technique of adiabatic data analysis by the ADaExpert program which utilizes several unique methods.

10. Kinetics-based simulation approach. More about applying simulation for evaluating reactive hazard of Li-ion battery (see abstract above)

This is the second part of study presented in the 8th newsletter. It shows the use of the kinetics for assessing the runaway hazard. One of the highlights is the very good accord of the CISP results with the runaway simulation implemented independently by the Kobelco Research Institute (Japan).

11. Reaction calorimetry (RC): types, simple theory and application for kinetic study (overview)

The newsletter contains description of the existing types of RC in compact form. The overview can be helpful in understanding principles of RC and in choosing the type of instrument most relevant for study of specific problem.

12. Do we know everything about DSC data? How to interpret DSC data when the overall heat depends on heating rate

The newsletter discusses one unusual case when the overall reaction heat varies with heating rate and reveals the origin of this phenomenon that can easily be considered as experiment's error.

13 Kinetics-based simulation of thermal explosion – some examples of experimental validation

Several cases when prediction of thermal explosion by kinetics-based simulation was verified by the large-scale explosive experiments are presented in this issue.

14 Simple theory of melting based on the DSC model or what we can learn from such experiments

This paper describes simple model of melting at linear heating and gives several useful recommendations..

15 Glass crucibles for calorimeters with the 3D Calvet-type sensors

The aim of this short newsletter is to share our experience in applying home-made sealed glass crucibles in DSC experiments.

16. ARKS TE software - purpose and features [DOI: 10.13140/RG.2.2.25521.10082](https://doi.org/10.13140/RG.2.2.25521.10082)

Introduction to the TSS-ARKS applications that support the kinetics-based simulation approach in mode details

17. Example of kinetic analysis of complex thermogravimetry data (A. Kossoy, A. Lopatin) [DOI: 10.13140/RG.2.2.16819.35364](https://doi.org/10.13140/RG.2.2.16819.35364)

Demonstration of what can be done by the model-based kinetic analysis method for evaluation of complex kinetics from TG data.

18. Kinetics-based simulation approach. Convenient way to take a closer look at TSS-ARKS software

Description of the video lessons that help a user to master the software.