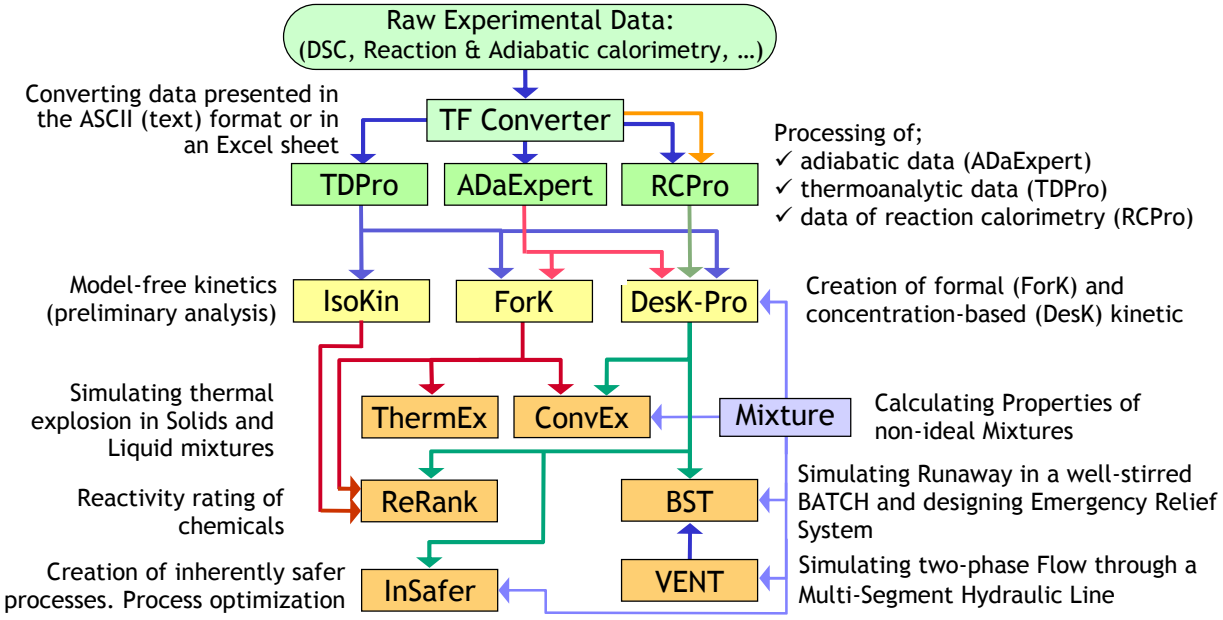
CHEMINFORM ST.PETERSBURG

Thermal Safety Software (TSS) series

Assessing Thermal Hazards of Chemical Processes and Products.

- TSS covers the entire spectrum from experimental study of a reaction and processing of experimental data to creation of a kinetic model to simulation of chemical reactors and runaways of various kinds
- TSS gives general solution of the crucial challenge of hazard assessment–the scale-up problem
- TSS components are interlinked to each other providing a unified analog-free system
- Each TSS application has a unique set of features that distinguishes it from other commercial offerings. TSS 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
- Detailed problems-solving Tutorials
- Complete set of user manuals
- Minimum hardware requirements: Pentium V, Windows 2000, XP, VISTA, 7

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193232, St. Petersburg, PO box 25, Russia. Tel /Fax +7 (812) 647 92 52;
E-mail: office@cisp.spb.ru; Web: http://www.cisp.spb.ru

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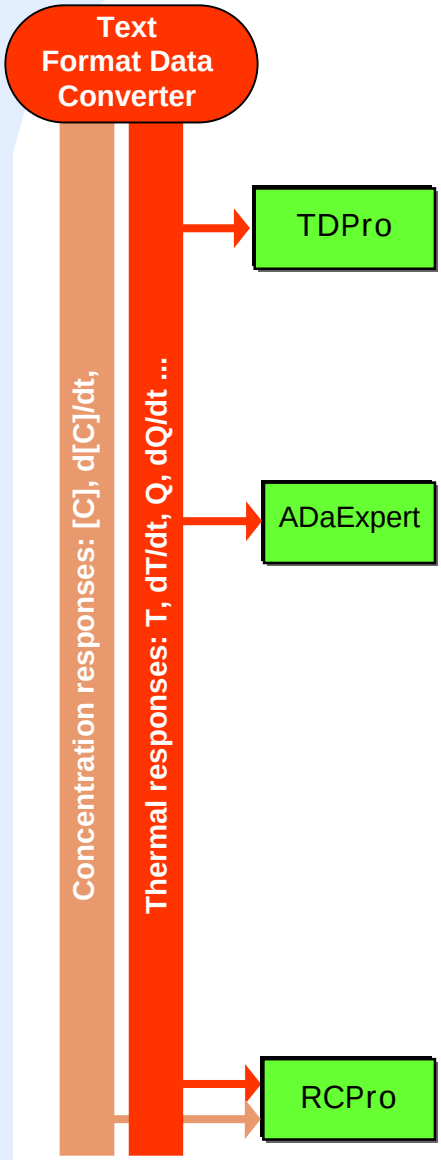
TSS applications for processing of experimental data



Thermal analysis data: DSC, HFC, TG, TDA, combined data:

- Correcting Data on Instr. Base Line
- Editing Data (deleting fragments, smoothing, thinning out)
- Reconstructing base line under peak
- Statistical analysis
- Reconstructing Sample Temperature
- Deconvoluting Data
- Determining specific heat, phase transition parameters, dynamic calibration

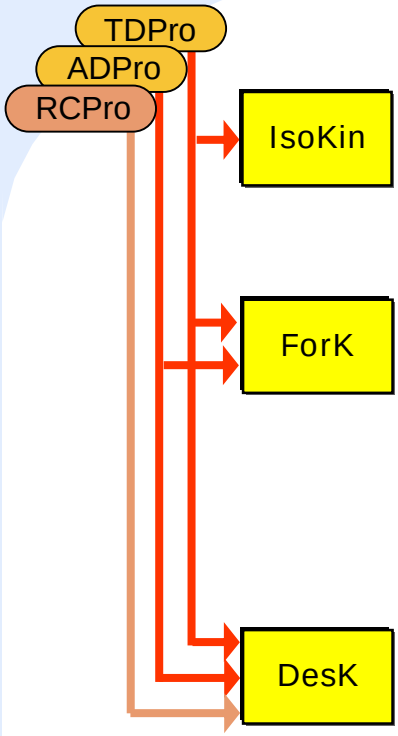
Adiabatic data analysis: ARC, VSP, Phi-Tec, DEWAR, RSST:

- Editing Data (deleting fragments, smoothing, thinning out)
- Calculating phi-factor
- Correcting Pressure Response
  - Pad gas pressure correction
  - Determining Antoine or August constants for Pv and correcting pressure response
- Determining the onset temperature
- Building complementary responses (gas & heat production, derivative responses
- Accounting for variable Cp, thermal expansion of sample and bomb
- Accounting for thermal initiation pre-history to evaluate initial sample state at onset temperature
- Evaluation of Simple Reaction Kinetics
- Advanced method for thermal inertia correction
- Estimation of Time to Maximum Rate
- Vent sizing, choice between Leung Omega method & ISO 4126-10

Reaction calorimetry data: RC-1, SIMULAR, others:

- Supports data of BATCH and semi-BATCH experiments
- Editing Thermal Data (deleting fragments, smoothing, thinning out)
- Reconstructing base line
- Correcting Pressure Response (same as in ADPro)
- Editing Concentration Data
- Building complementary responses

TSS applications for kinetics evaluation



Isoconversional kinetics: Fast preliminary kinetic analysis including:

* 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)

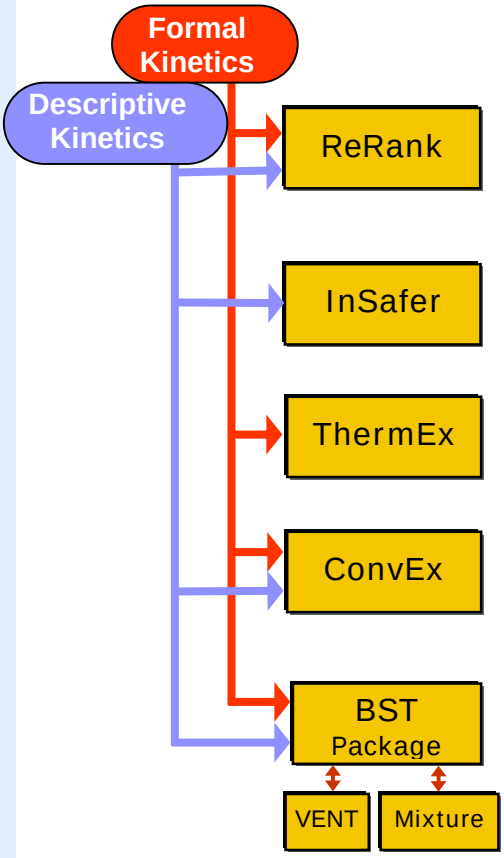
Formal conversion-based models:

* 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 and CSTR reactors under variety of thermal modes
* Calculation of hazard indicators (adiabatic TMR, thermal stability)

TSS applications for Reaction Hazard Assessment



Assessing Reactivity:

* Automatic determination of NFPA reactivity number – standard and advanced methods
* Automatic determination of adiabatic TMR & TER
* Automatic estimate of Thermal Stability (TCL)

Design of Inherently Safer Processes:

* Providing safety of normal operational mode
* Providing maximal possible safety in case of accident
* Analysihg 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

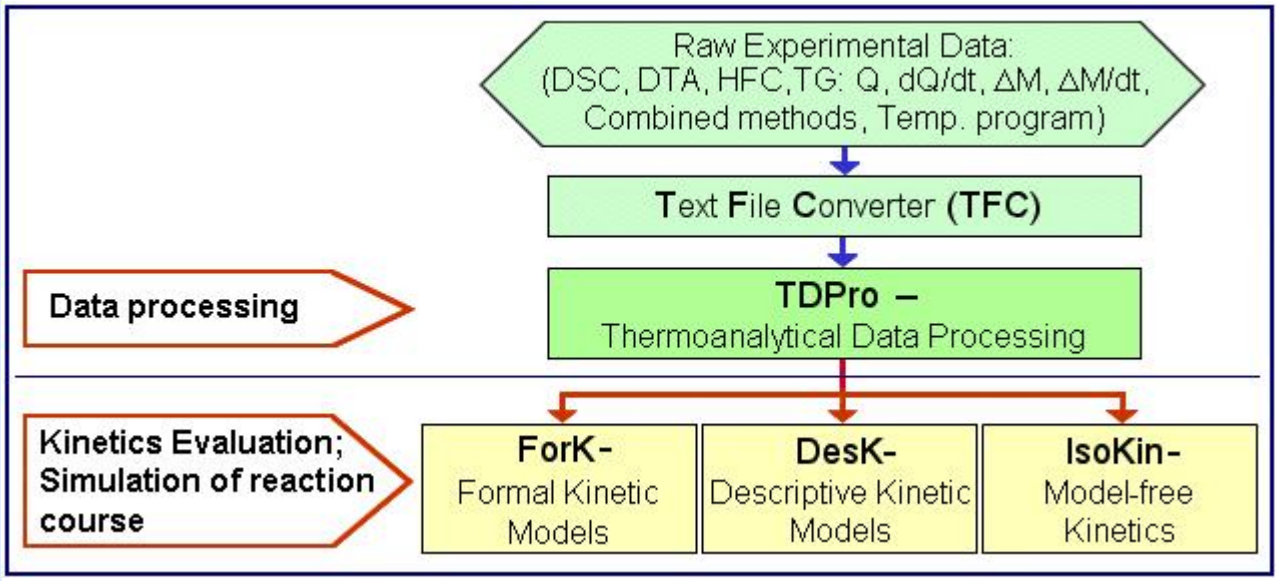
The TSS series includes more than 12 applications. In many cases there is no need to use all of them. Moreover, though the primary aim of TSS is to help in reaction hazard assessment its components can be successfully used in various researches that are not related with hazards. We can offer several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

You won't finde here the detailed specifications of the programs that compose the sub-sets proposed. We mentioned only some features that are relevant to the area of application. More detailed description of every program can be found in the brochure "TSS-specifications".

The sub-set for thermal analysis

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

It consists of TDPro, ForK and/or DesK and/or IsoKin.



TDPro 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, parameters of phase transition, thermal conductivity of liquids. The auxiliary Text File Converter program allows simple method for data conversion so that TDPro can be used in combination with any thermal analytical instrument.

The line of programs **ForK/DesK/IsoKin** allows evaluation of reaction kinetic models 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 these programs have powerful modules for simulation of reaction course under various conditions. Therefore they can be successfully used for solving variety of practical problems from analysis of thermal stability to estimation of thermal mode of a reactor.

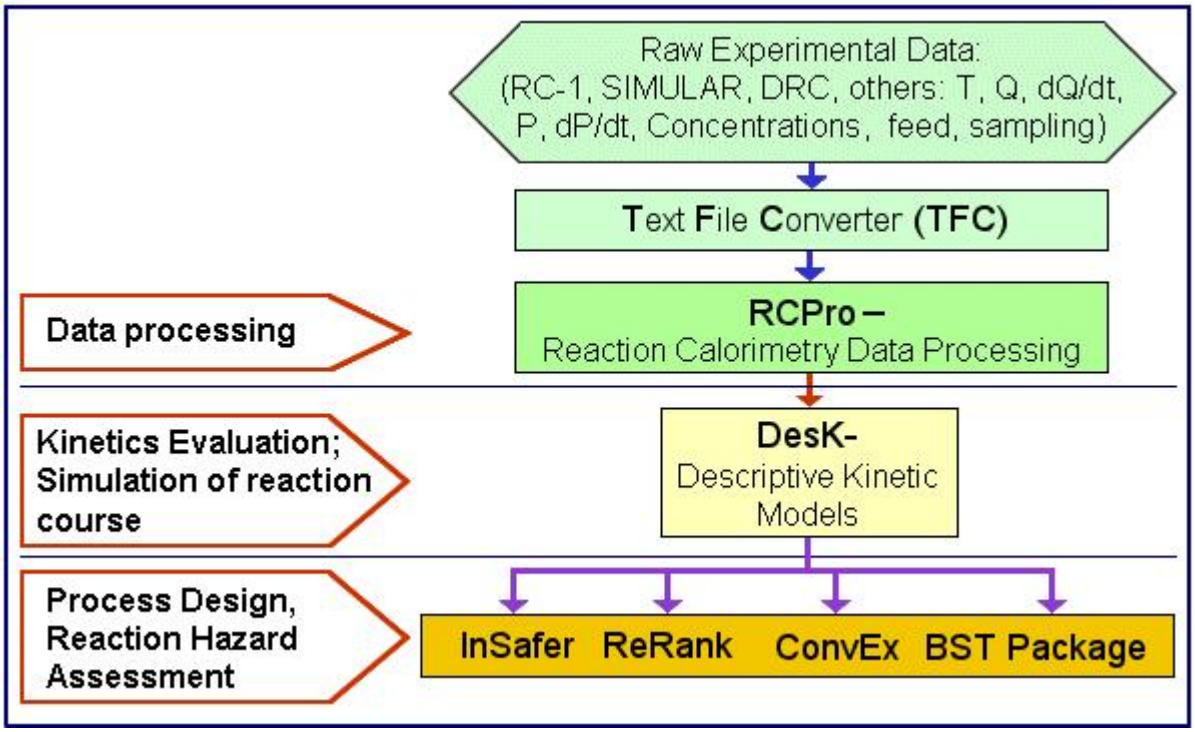
ForK is designed for creation of conversion-based complex multi-stage formal models.

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

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

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 RCPro, DesK, InSafer and/or ReRank and/or ConvEx and/or BST Package.



RCPro 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 Text File Converter program allows simple method for data conversion. RCPro can be used in combination with any available reaction calorimeter.

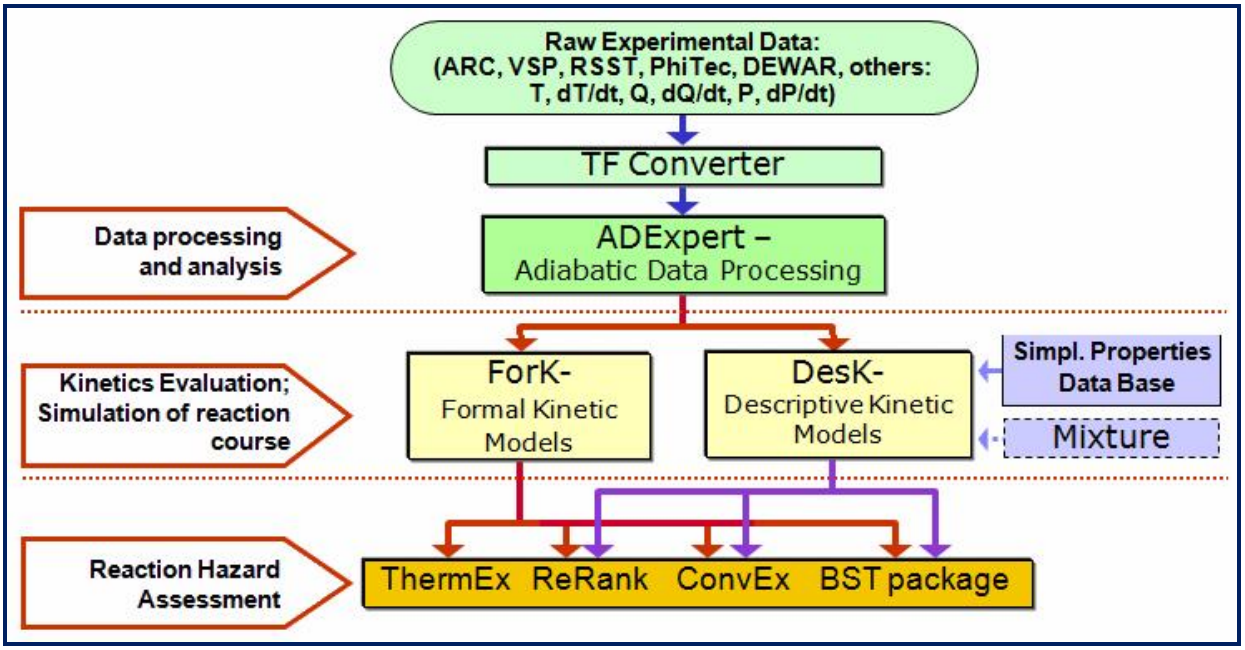
DesK allows creation of complex multi-stage concentration-based reaction models. The bunch of the state-of the-art math methods for numerical integration of non-linear reaction models and non-linear optimization in conjunction with calculation of variable physical-chemical properties of mixtures makes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

The line of programs **InSafer/ReRank/ConvEx/BST** allows solving various practical problems. The choice depends on the kind of investigations carried out in the laboratory.

InSafer 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. InSafer 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 ADaExpert, ForK and/or DesK, and the pack consisting of ThermEx, ReRank, ConvEx and BST.



ADaExpert 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 Text File Converter program allows simple method for data conversion so that ADaExpert 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 advances method for thermal inertia correction, adiabatic TMR calculation and vent sizing.

ForK and/or 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 ForK would be the right choice. If the laboratory is involved in process safety studies then we would recommend considering DesK as a candidate. The pair ForK + DesK covers a wide range of problems and therefore provides maximal flexibility.

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

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

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

ThermEx and **ConvEx** are for simulation of thermal explosions in solids and liquids.

ReRank provides easy and fast determination of hazard indicators of chemicals.

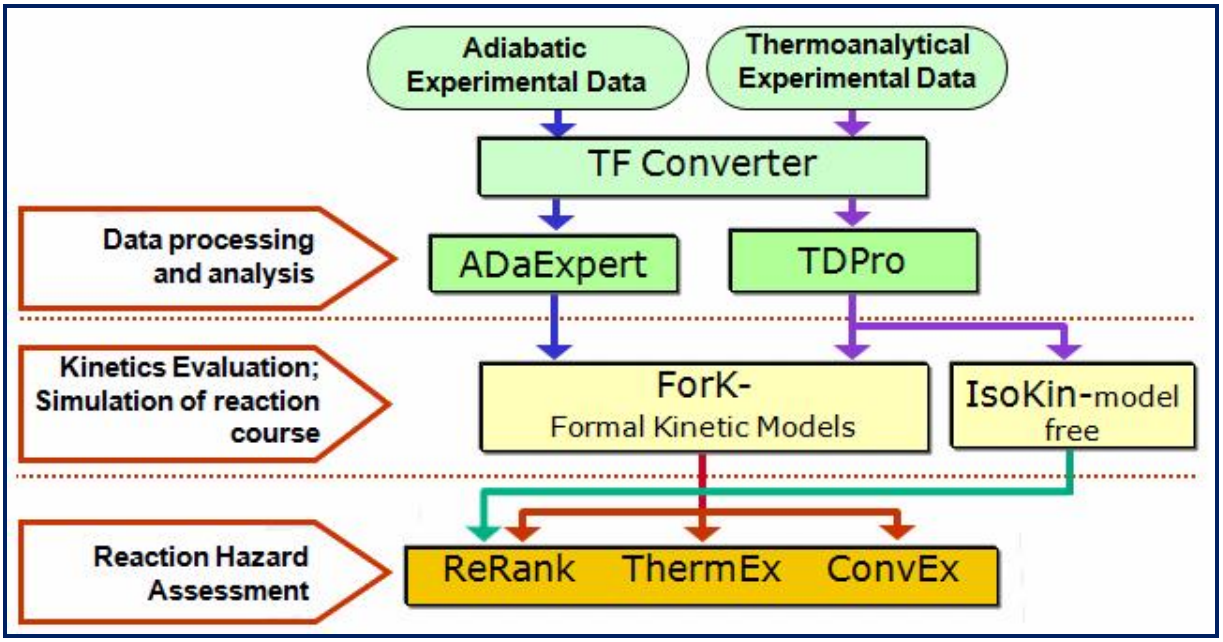
BST package is intended for design of emergency relief systems.

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 ReRank- ThermEx-ConvEx 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 ADaExpert, TDPro, ForK and IsoKin, and ReRank, ThermEx and ConvEx.



TDPro and **ADaExpert** support all necessary types of data processing for data of thermal analysis and adiabatic calorimetry. The auxiliary Text File Converter program allows simple method for data conversion so that TDPro and ADaExpert can be used in combination with any thermal analytical and adiabatic instrument respectively.

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

IsoKin 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 **ForK**. These models are the basis for assessing hazard by applying the last group of programs.

ReRank provides easy and fast determination of hazard indicators of chemicals whereas

ThermEx and **ConvEx** provide in-depth analysis of thermal explosion hazards of solid and liquid chemicals.