

A computerized system for research into the thermal safety of chemical processes

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Abstract

Ensuring the thermal safety of chemical processes is an important practical problem because of the possible development of thermal explosion caused by the heat evolved during the chemical processes.

A computerized system developed for solving this complicated problem is described, based on the range of Setaram thermoanalytical and calorimetric devices. The structure, purpose and possibilities of the system are considered. Methodological questions of kinetic experiments, kinetic analysis, thermal explosion simulation and organization of software are also discussed.

INTRODUCTION

Ensuring the thermal safety of chemical processes, i.e. the possible development of thermal explosion due to the heat evolved during the processes, is an important practical problem. The importance of research into thermal safety arises in

- (i) the determination of safe technological regimes for exothermic chemical processes in the processing unit;
- (ii) the probability evaluation of thermal explosion development in processing units because of various deviations from the correct course of the technological process;
- (iii) the determination of safe conditions of storage, transportation and application of chemical products that are inclined to exothermic decomposition (explosives, fertilizers, etc.).

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Dedicated to Professor Joseph H. Flynn in honour of his 70th birthday.

The current approach to the solution of the thermal safety problem is based on the use of suitable experimental methods and methods of mathematical simulation; thus, the various tasks associated with safety evaluation can be dealt with most effectively with maximum reliability, and the time necessary for carrying out the research can be reduced. An application of this approach is the computerized system for research into the thermal safety of chemical processes (system THERMAL SAFETY). The structure and main functions of this system, developed in our institute [1–3], are discussed in this article.

FUNCTIONS AND STRUCTURE OF THE COMPUTERIZED SYSTEM

The system THERMAL SAFETY is a complex of interconnected experimental techniques, methodological means, computers and software, which are included in the automated technology of thermal safety research.

The probability of thermal explosion is mainly determined by the kinetics of the chemical process, the construction and size of the processing unit, and the technological parameters of its functioning. Therefore the system must ensure that the following tasks are completed:

- (i) the experimental investigation of chemical reaction kinetics and the formulation of its kinetic description (kinetic analysis);
- (ii) the construction of a mathematical model of the chemical process, including, as its constituent part, the kinetic description of the process;
- (iii) the analysis of the increased probability of thermal explosion during the chemical process being simulated.

The experimental kinetic research, kinetic analysis and explosion simulation are all combined in the system THERMAL SAFETY into one iterative procedure. In accordance with the tasks to be solved, the system includes the following functional subsystems (SS) (see Fig. 1):

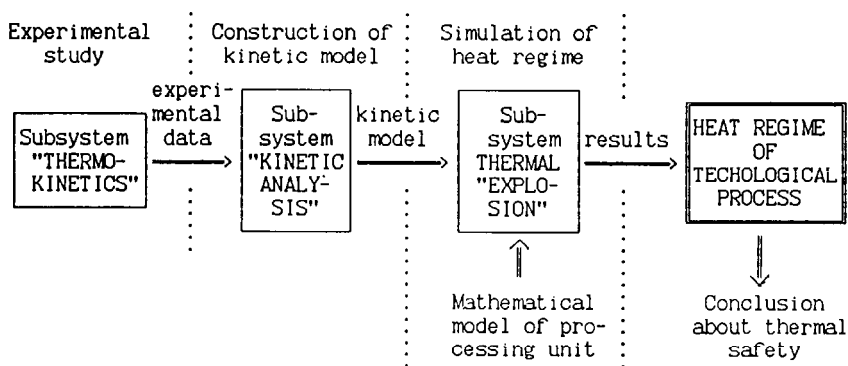


Fig. 1. Structure of the system THERMAL SAFETY and scheme of information flow.

(i) the subsystem for thermo-kinetic research (SS THERMOKINETICS) which is intended for experimental study of heat-evolving kinetics in chemical processes;

(ii) the subsystem for kinetic analysis (SS KINETIC ANALYSIS) the purpose of which is the formulation of mathematical descriptions of chemical reactions, based on experimental data, obtained using SS THERMOKINETICS;

(iii) the subsystem for thermal explosion simulation (SS THERMAL EXPLOSION) which is intended for calculation of the thermal regimes of the processing units and for determination of the conditions ensuring the thermal safety of the processes to be carried out.

The subsystem THERMOKINETICS

Technical base of the subsystem

The investigation of the heat-evolving kinetics accompanying a chemical process is one of the main stages in thermal safety research. Thermal analysis methods, differential scanning calorimetry, micro-calorimetry, etc., are especially adapted for this purpose.

The choice of suitable devices from the various instruments currently available is defined by the type of material being examined and by the required range of experimental conditions. In applications of the THERMAL SAFETY system, a range of Setaram thermoanalytical instruments, including the differential scanning calorimeter DSC-111, the microcalorimeter C-80 and the thermoanalyser TG-DSC-111, is used; this makes it possible to carry out kinetic investigations of the heat evolution and mass changes over a wide range of temperatures (170–1000 K), pressures (up to 1.5×10^7 Pa) and in different gaseous atmospheres. The set of experimental reactive cells allows simulations of the different ways in which chemical processes can proceed, including forced agitation (in a C-80 calorimeter).

Thermoanalytical methods yield data relating only to the overall change in the brutto characteristics of the process (heat evolution, mass loss, gas evolution, etc.). Therefore, chromatography and chromatography coupled with mass spectrometry are widely used in our kinetic investigations for obtaining more detailed information on the mechanisms of chemical reactions.

It should be mentioned that the Mettler RC-1 reaction calorimeter can, in many cases, be a very useful addition to the set of instruments described above. For experiment automation, IBM-compatible PC-AT computers are used.

Methodological supplement of the subsystem THERMOKINETICS

The creation of this subsystem required considerable development of the methodologies of thermo-kinetic research. Some problems connected with

the application of the thermoanalytical methods are briefly discussed below.

In kinetic investigations, it is essential to have a uniform distribution of temperature and of concentrations of reagents in a sample (thermophysical and concentrational correctness of an experiment [4,5]). We have classified different techniques for correct experimental procedures and have developed experimental and calculating methods for testing these [6].

The temperature of the reacting system, which is one of the fundamental experimental parameters, is not measured directly as a rule. In order to obtain reliable estimations of this quantity, we have developed a method for calculating the sample temperature from measurements of the calorimetric signal. It should be noted that the temperature estimations obtained are also related to the simultaneous calorimetric and thermo-weight experiment.

At present, complicated, partially linear, heating laws are frequently used; for instance, the combination of sections with various constant heating rates (any of the sections may be isothermal). Analysis of the suitability of these heating laws was made on the basis of the physical model of a heat flux calorimeter [6]. The conditions providing correctness of kinetic experiments were also determined.

The measuring calorimetric cell itself introduces dynamic distortions because of heat inertia, which leads to a significant deformation of the kinetic curve in some cases. Even small distortions may lead to considerable errors in the estimation of kinetic model parameters. Therefore, correction of distortions having an amplitude 3–5% from the heat evolving rate, diminishes by half the error in the determination of the kinetic parameters. We have developed a procedure for deconvolution of experimental data for their correction [7]; examples are presented in Fig. 2.

Data error is an important characteristic of any data. It is defined by statistics processing of the results of parallel experiments. For this purpose we have developed a special algorithm based on the random data analysis theory [8] which allows the data to be estimated with quantitative reproducibility and an average kinetic curve and error corridor to be determined [9].

Software for the subsystem THERMOKINETICS

Software for the thermokinetic experiment is produced from the methodological developments; it consists of an application package THERMAL EXPERIMENT to be run on IBM-compatible PC-XT/AT computers, which includes the program modules CONTROL MODULE, DATA BASE, INITIAL PROCESSING and PHASE TRANSITIONS.

CONTROL MODULE automates all operations associated with carrying out the experiments, such as experiment control, data collection and storage, producing of static and dynamic DSC, DTA calibrations for the Joule

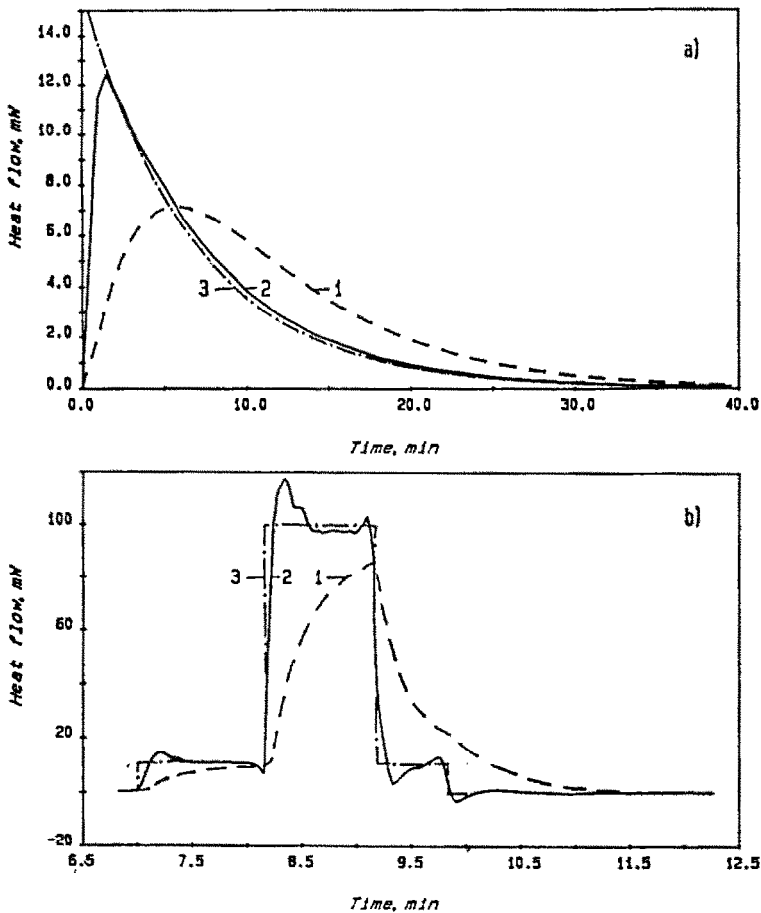


Fig. 2. Deconvolution of calorimetric data. 1, experimental curve; 2, deconvoluted curve; 3, original heat flow. (a) C-80, isothermal heating law. (b) DSC-111, linear heating law.

effect or on phase transitions in standard substances, etc. CONTROL MODULE controls the Setaram instruments in various configurations. It may also be used for automation of other DTA, DSC or TG instruments.

The DATA BASE module is for storing the experimental data, and the initial processing of results and experimental conditions.

The INITIAL PROCESSING module is used for obtaining the rate of heat evolution and mass loss as functions of time according to signals being measured. Thus all necessary functions for initial data processing can be performed [3].

The PHASE TRANSITIONS module allows the determination of the temperature and enthalpy of phase transitions in solids, and it provides the determination of calibration characteristics of DTA and DSC instruments (calibration on phase transitions).

The subsystem KINETIC ANALYSIS

The subsystem KINETIC ANALYSIS formulates mathematical descriptions of the chemical reactions from the experimental data obtained by means of the subsystem THERMOKINETICS.

For this purpose kinetic models are used which are presented by systems of ordinary differential or algebraic equations. Multi-response models of this type make it possible to simulate the kinetics of the changes in the characteristics of individual reactions (heat evolution, mass loss, concentrations, gas evolution) and their combinations.

Depending on the level of the detailed mechanism of the chemical reaction, the models are divided into two groups: phenomenological and generalized formal kinetic models.

Phenomenological models are constructed on the basis of an assigned mechanism of a chemical reaction

$$\frac{dC_i}{dt} = \sum_{j=1}^M \nu_{ij} K_j \prod_{n=1}^N C_n^{|\nu_{nj}|} \quad (1)$$

where C_n is the concentration of reagent i ($1 < i, n < N$), $K_j = K_{0j} \exp(-E_j/RT)$ is the reaction rate constant of stage j ($1 < j < N$) and ν_{ij} are stoichiometric coefficients.

The system may be expanded by the heat balance equation

$$\frac{dQ}{dt} = \sum_{j=1}^M Q_j^\infty K_j \prod_{n=1}^N C_n^{|\nu_{nj}|} \quad (2)$$

where Q_j^∞ is the heat effect of the j th stage.

For construction of widely used, generalized, formal kinetic models with complicated structures, we have suggested a procedure of automated model synthesis from a standard set of kinetic equations describing separate brutto stages of the reactions. There is a common form of model structure

$$\begin{aligned} \frac{dS}{dt} &= \sum_{i=1}^w \sum_{j=1}^{r(i)} S_{ij}^\infty \left(\frac{d\alpha_i}{dt} \right)_j \\ \frac{d\alpha_i}{dt} &= \sum_{i=1}^{r(i)} \left(\frac{d\alpha_i}{dt} \right)_j \quad \left(\frac{d\alpha_i}{dt} \right)_j = f_{ij}(\alpha_i) K_{ij} \end{aligned} \quad (3)$$

where S is the response, α_i the degree of conversion in the i th reaction, $(d\alpha_i/dt)_j$ the rate of the j th parallel stage in the i th reaction, S^∞ the specific value of the response at stage j at $\alpha_{ij} = 1$, $K = K_0 \exp(-E/RT)$ is the rate constant of a stage, $T = T(t)$, the temperature of the reacting system, w the number of reactions and r the number of parallel stages; K_0 , E , n , m , S^∞ and α_0 are the model's parameters.

Some functions from a standard set of kinetic equations are also presented

$$\begin{aligned}
 f(\alpha) &= (1 - \alpha)^n && n\text{-th order reaction} \\
 f(\alpha) &= \alpha^n && \text{degree reaction} \\
 f(\alpha) &= (1 - \alpha)(\alpha + \alpha_0) && \text{simple autocatalysis} \\
 f(\alpha) &= \alpha^n(1 - \alpha)^m && \text{autocatalytic reaction} \\
 f(\alpha) &= (1 - \alpha)(-\ln(1 - \alpha))^n && \text{solid-state reaction} \\
 &&& \text{(Avrami–Erofeev model)}
 \end{aligned} \tag{4}$$

Brutto multi-stage independent, parallel reactions, and their combinations can be described by means of various combinations of the basic equations. Structural and parametric identification is carried out during the inverse task, solving from the experimental data after initial processing.

The data may be heterogeneous, consisting of kinetic curves, representing changes of any reacting system responses or rates of response changes with time (integral or differential form); sets of response values, corresponding to parallel runs; and omitted observations.

The possibility of simultaneous utilization of experimental data obtained in different temperature–time modes is the unique property of the model.

Methodological provision of kinetic analysis

The important problem of kinetic analysis is the mathematical correctness of inverse task positing, i.e. the existence and single value of the inverse task solution for an arbitrary set of experimental data and solution stability by small data variations [10]. The existence of a solution is guaranteed if the number of parameters of the model is a finite quantity and if their determination region is defined. But further analysis is required for the determination of a single-value solution and its stability. In practice, the task positing correctness may only be confirmed after determining the point estimation of the vector \bar{P} of the parameters and its analysis.

Parametric identification, i.e. evaluation of the parameters of a given kinetic reaction model, is based on the least-squares method (LSM) [11]. The LSM does not require a knowledge of the distribution of observations and is well adapted for realization on computers. This method is useful for processing of heterogeneous experimental data and permits determination not only of the kinetic parameter (activation energy, pre-exponent, reactions order, etc.) but also of such factors as the initial values of conversion degree, concentrations, etc. In non-linear models, the application of non-linear programming methods [12] is required for utilization of the LSM. Based on our experience, we chose a modified Gauss–Newton method (numerical realization [13]), which gives the best results for the models

mentioned above. The main purpose of this method is the linearization of the determined component $f(\bar{P})$ of the observation model

$$y = f(\bar{P}) + \varepsilon$$

where y is the reacting system response and ε the experimental error.

Examples of kinetic model parametric identification are presented in Fig. 3.

The causes of multi-valued solutions are the model structure, the deficiency of experimental data and their error. Cases of global and local multi-values are distinct [14].

A general mathematical method has not been formulated for global multi-valued solutions; therefore, the corresponding verification is made using our software by means of experimental calculations.

We applied [15] a method of weighted Jacoby-matrix singular analysis [16] for a posteriori determination of local multi-values. This method also allows the degree of solution stability with respect to small experimental data variations to be determined.

The estimation of errors in the parameters may be determined using probability methods [11] or the Bayes approach [17]. But correct solution of this problem is only possible by means of robust methods [18] because the distribution law of the observation errors is usually unknown. We propose to use the envelope surface for permissible values of the parameters, region D , characteristic for robust errors

$$D = \left\{ \bar{P} \mid \text{abs}(f(\bar{P}) - y) < E_m \right\}$$

where E_m is the maximum value of experimental error.

Region D may be of large dimension and complex configuration because of the correlation between the estimations of the parameters. Its two-dimensional cross-sections allow the solution error to be estimated to a certain extent.

Software for the subsystem KINETIC ANALYSIS

Functions of the subsystem `KINETIC ANALYSIS` are contained in the application package `MACROKINETICS` `GUI` on PC-AT computers. The package consists of the program modules `DATA BASE`, `KINETIC ANALYSIS` and `DIRECT TASK`.

The `DATA BASE` module is used for experimental data, kinetic models and storage of parameters sets, and provides all the necessary procedures connected with adding, search, looking through, editing and deleting information.

The kinetic description of the chemical reaction corresponding to the experimental data is obtained by means of the `KINETIC ANALYSIS` module. This module makes it possible to estimate all or only part of the parame-

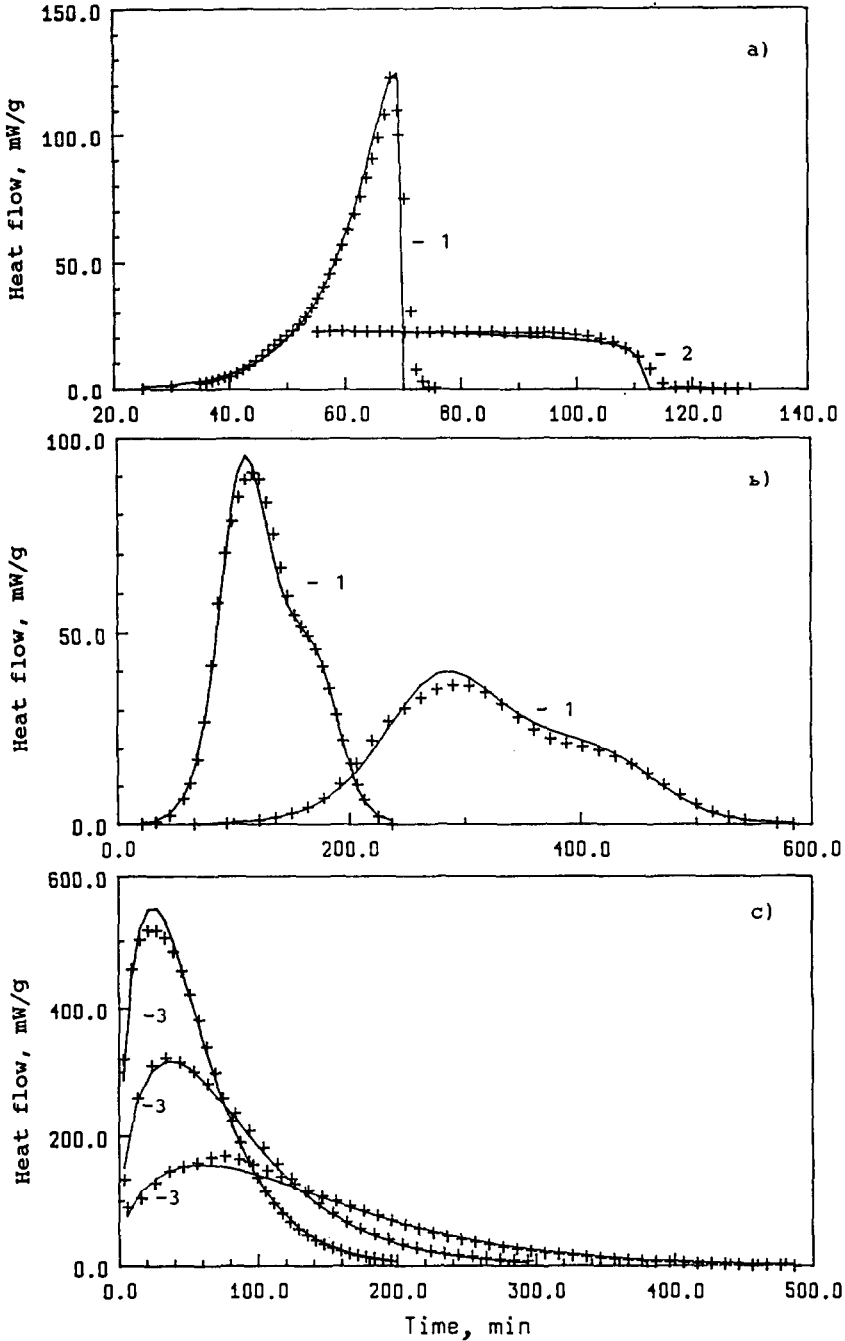


Fig. 3. Examples of parametric identification: +, experimental curves, —, results of kinetic analysis. 1, linear heating law; 2, isothermal part of combined heating law; 3, isothermal condition. (a) Thermal decomposition of $\text{Na}_2\text{CO}_3 \cdot 1.5\text{H}_2\text{O}$, model of n -th order reaction. (b) Liquid phase reaction: 1,2-dichloroethane + ethylenediamine, model of sequential reactions. (c) Liquid phase reaction: 1,1-dimethylhydrazine + ethyl oxide, model of full autocatalysis.

ters of the kinetic model, to determine an estimation of errors in the parameters, to carry out computing experiments, etc.

The **DIRECT TASK** module is used for calculation of the response of the reacting system, according to known kinetic reaction descriptions and reaction conditions in the absence of concentration and temperature fields. Calculations are made analytically or by one of the standard numerical integration methods.

Estimation of the subsystem's metrological characteristic

A significant problem associated with employment of the system is the estimation of the metrological characteristics of the whole system and their subsystems. The well-known error-estimation method by means of standards cannot be applied in kinetic research because of the absence of standard reacting systems, the wide range of the physicochemical properties of the reagents and the variety of reaction conditions.

We have worked out a method of simulating experiments [19] which can be regarded as a possible solution of this problem for calorimetric research.

The simulating experiment makes it possible to define the heat process in the DSC cell with a given heat-evolution law in conditions as close as possible to the experimental ones. The heat evolved is provided by a microheater inserted in an experimental cell or by a standard calibration cell included in the set of heat-flow calorimeters.

Simulation of the desired heat-evolution law is ensured by using computer-controlled power supply to the microheater. Means are proposed for simulating thermophysical conditions of real kinetic experiments.

Metrological characteristics are estimated by comparison of data-processing results with known parameters of determining heat processes.

For calorimetric researches, simulating experiments yield:

- static and dynamic calibrations of a calorimeter;
- an estimation of the correctness of algorithms used for initial processing of experimental data;
- the determination of measurement errors for heat evolution rates and heat effects;
- an estimation of the experimental reproducibility.

For kinetic researches using DSC, simulating experiments make it possible to:

- simulate the heat evolution corresponding to the required kinetic law;
- estimate the metrological characteristics of the kinetic experiment;
- estimate the influence of experimental errors on the accuracy of the kinetic parameters determined by kinetic analysis of simulating experimental data without model mistake.

It must be pointed out that the subsystem **KINETIC ANALYSIS** can be used to execute a computing experiment which may also be used for subsystem

self-testing. Such an experiment is often useful for the design of additional or control runs during kinetic research.

The subsystem THERMAL EXPLOSION

The subsystem THERMAL EXPLOSION is intended for the mathematical simulation of thermal explosion in reactors with distributed parameters; it allows calculations to be made for reacting systems with heat transfer due to heat conductivity. The use of effective heat conductivity also makes it possible, in some cases, to simulate systems in which natural convection takes place.

An analysis of thermal explosion development can be made for reacting volumes of various shapes. The volume may be surrounded by a multi-layer enclosure and may have a set of internal inert partitions with various thermophysical properties.

The main purpose of thermal explosion simulation is the determination of critical conditions (size of reacting system, environment temperature, induction period), i.e. the conditions separating fields of explosive and non-explosive processes. This determination is carried out by simultaneous solution of partial differential equations for the heat conductivity process and chemical reaction

$$\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial T}{\partial r} \left(r \lambda \frac{\partial T}{\partial r} \right) + \frac{\partial T}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + W \quad (5)$$

where W is the rate of heat evolved as determined by kinetic models (2), (3), or (4), T is the temperature, t the time, r and z are space variables and C_p , ρ and λ are the heat capacity, density and heat conductivity of the substance.

Initial conditions for system (5) are $t = 0$; $T(r, z) = T_0(r, z)$; $\alpha_i(r, z) = 0$ (for kinetic model (4)) or $C_i(r, z) = C_{i0}(r, z)$ (for kinetic models (2) and (3)).

Calculations can be carried out for boundary conditions of the first, second and third type on the surface of reacting volumes. The temperatures or heat flows on the surface may be presented as given functions of time.

Numerical solution methods

During the description of the subsystems, we have stressed the choice of the optimal method for problem solving. Specifically, the chosen method must provide the most rapid and exact determination of the induction period because this is one of the most important characteristics of thermal explosions.

The equation system (5) is generally solved using a uniform, conservative σ -parametric difference scheme, with splitting on physical processes and space variables [20].

Three schemes of this type are known [21,22]

(1) a linearized scheme with increments of functions;

(2) a scheme in functions, with iteration of the chemical stage by Newton's method;

(3) a scheme based on Gear's method with the second order of accuracy.

These schemes are absolutely stable for $\sigma \in (0.5; 1)$ and have a second order of approximation for space and a first one for time at uniform splitting.

According to the first and second schemes, the system (5) is written in difference form after substitution of differential operators for the appropriate difference forms as

$$\frac{\bar{X}^{n+1} - \bar{X}^n}{h_t} + L_2(\sigma \bar{X}^{n+1} + (1 - \sigma)\bar{X}^n) = \sigma \bar{F}^{n+1} + (1 - \sigma)\bar{F}^n \quad (6)$$

where $\bar{F} = \bar{F}(\bar{X})$ is the right-hand-side vector, \bar{X} is the solution vector, $L_2 = L_r + L_z$ where L_r and L_z are second-order difference operators approximating the differential operators in system (5), h_t is a step for time and n is the number of time layers.

The first scheme, after splitting on physical processes and space variables, leads to the linear equation system

$$\left\{ \begin{array}{l} (E + \sigma h_t L_1) \delta X_{ij}^{n+1/3} = -h_t (L_2 X_{ij}^n - F_{ij}^n) \end{array} \right. \quad (7)$$

$$\left\{ \begin{array}{l} (E + \sigma h_t L_r) \delta X_{ij}^{n+2/3} = \delta X_{ij}^{n+1/3} \end{array} \right. \quad (8)$$

$$\left\{ \begin{array}{l} (E + \sigma h_t L_z) \delta X_{ij}^{n+1} = \delta X_{ij}^{n+2/3} \end{array} \right. \quad (9)$$

$$\left\{ \begin{array}{l} X_{ij}^{n+1} = X_{ij}^n + \delta X_{ij}^{n+1} \end{array} \right.$$

where $L_1() = -\partial \bar{F} / \partial \bar{X}$, E is the unit matrix and i, j are coordinates of space grid junctions.

The second scheme leads, after splitting, to the equation system

$$\left\{ \begin{array}{l} X_{ij}^{n+1/3} - X_{ij}^n = h_t (\sigma F_{ij}^{n+1} + (1 - \sigma) F_{ij}^n) \end{array} \right. \quad (10)$$

$$\left\{ \begin{array}{l} (E + \sigma h_t L_r) X_{ij}^{n+2/3} = X_{ij}^{n+1/3} - h_t (1 - \sigma) L_2 X_{ij}^n \end{array} \right. \quad (11)$$

$$\left\{ \begin{array}{l} (E + \sigma h_t L_z) X_{ij}^{n+1} = X_{ij}^{n+2/3} \end{array} \right. \quad (12)$$

The non-linear equation system (10) is solved by Newton's method.

According to the third scheme [22], the equation system (5) is written in difference form as

$$\frac{1.5 \bar{X}^{n+1} - 2 \bar{X}^n + 0.5 \bar{X}^{n-1}}{h_t} + L_2(\sigma \bar{X}^{n+1} + (1 - \sigma)\bar{X}^n) = \bar{F}^{n+1} \quad (6a)$$

and we obtain, after splitting, the linear equation system

$$\left\{ \begin{array}{l} (E + 2/3h_t L_1) \delta X_{ij}^{n+1/3} = 1/3(X_{ij}^n - X_{ij}^{n-1}) + 2/3h_t F_{ij}^n \\ X_{ij}^{n+1/3} = X_{ij}^n + \delta X_{ij}^{n+1/3} \end{array} \right. \quad (13)$$

$$\left\{ \begin{array}{l} (E + 2/3\sigma h_t L_r) X_{ij}^{n+2/3} = X_{ij}^{n+1/3} \\ (E + 2/3\sigma h_t L_z) X_{ij}^{n+1} = X_{ij}^{n+2/3} \end{array} \right. \quad (14)$$

$$\left\{ \begin{array}{l} (E + 2/3\sigma h_t L_r) X_{ij}^{n+2/3} = X_{ij}^{n+1/3} \\ (E + 2/3\sigma h_t L_z) X_{ij}^{n+1} = X_{ij}^{n+2/3} \end{array} \right. \quad (15)$$

The linear algebraic equation systems (7) and (13) are solved by Gaussian elimination with partial pivoting. The Thompson algorithm is used for tri-diagonal solution of the linear algebraic equation systems (8) and (9), (11) and (12), and (14) and (15).

A comparison of the considered schemes was carried out by calculation using a set of various tests. Analysis of its results shows that the scheme based on Gear's method is the optimal one because it allows the induction period to be determined with the minimum calculating time and provides the required accuracy of temperature and concentration distribution calculation. Therefore we have used this method in the subsystem THERMAL EXPLOSION. Some examples of its application are presented in Fig. 4.

It should be noted that the specialized subsystem is now suitable for mathematical simulation of reacting systems in which natural convection takes place.

Software for the subsystem THERMAL EXPLOSION

Functions of the subsystem THERMAL EXPLOSION are contained in the application package THERMAL EXPLOSION run on PC-AT 386/486 computers. This package is fully compatible with the module DATA BASE of the subsystem KINETIC ANALYSIS and uses the same model structures.

Organization of system software

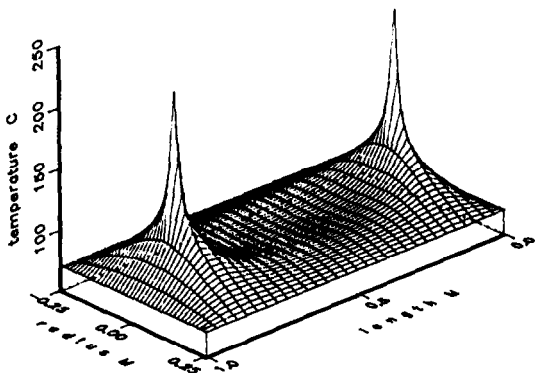
The software works under the MS-DOS operation system (version 3.3 and higher). Programming languages C, FORTRAN and ASSEMBLER were applied for software creation.

The software makes it possible to use all its features without specialized knowledge of programming, computing mathematics or mathematical methods of chemical kinetics.

The interactive mode of the packages greatly simplifies their use without universal instruction demands. Moreover this mode gives the opportunity of uniting the formalized methods of data processing with the researcher's experience and intuition, allowing him to influence the problem solving.

The interactive mode of the packages is created using the hierarchical "menu" type. All the questions included in "menu" are provided with replies where necessary. The interactive mode makes it possible to accom-

Time of the process (h:m:s) = 105: 1 : 44 (a)



Time of the process (h:m:s) = 105: 43 : 32 (b)

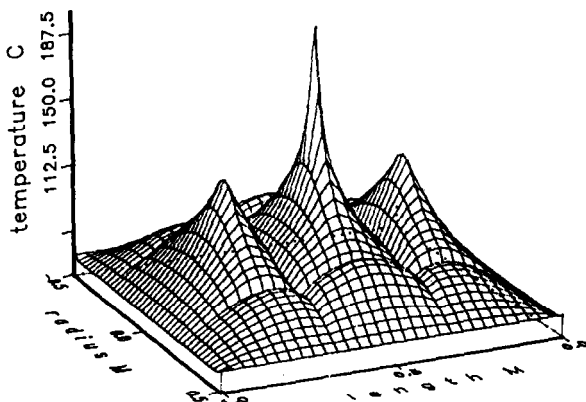


Fig. 4. Examples of thermal explosion simulation. Temperature field in reacting system of cylindrical shape; kinetic model of full autocatalysis reaction. (a) Without inert partitions. (b) With one coaxial and two transverse partitions.

plish syntax and context control, if possible. The researcher may use “help” when difficulties are encountered.

The graphical display of data provides all obvious ways of information presentation, facilitates the analysis of results and makes it easier to draw conclusions.

The data bases of the application packages are fully compatible, so that packages may be applied using either one or two levels of the system’s computer facility. In the last case the informational connection between the computers is easily provided by means of diskettes.

It must be pointed out that the applications packages may be used together or independently.

CONCLUSIONS

The system THERMAL SAFETY has been in use over several years. Its possibilities and fields of application expand continually. Some examples of its employment include: determination of safety regimes for the functioning of the vaporizer used in hydrogen peroxide concentration; thermal safety research into the storage of ethyl oxide and synthetic detergent based on sulfamic acid; thermal stability investigation of bleach, etc.

The accumulated experience of operation of the system in our institute confirms its expediency and its effectiveness in reducing the time spent in research, and in producing results of high quality and reliability.

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