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# EFFECTIVE ALGORITHMS FOR SOLVING COEFFICIENT PROBLEMS OF HIGH ACCURACY ORDER

*Annotation. In order to researh the materials thermophysical properties by the inverse methods, a corresponding class of mathematical models is derived. The processing procedure for simulation models is reduced to extreme formulation, that allowed to develop effective algorithms for solving coefficient problems of arbitrary accuracy order. The package of applied programs for solving coefficient problems of thermal conductivity by simulation modeling methods is developed. The package is made on the bases of the object-oriented programming requirements. The simulation procedure was based on a multiprocessor computing system application. The test problems solution results are presented on the basis of the proposed approach.*

*Key words: coefficient problems, extreme formulation, simulation models, heat conduction, heat transfer.*

## Introduction

When analyzing heat transfer through heat conduction, the solution results accuracy of a given problem can greatly be affected due to a lack of information on thermophysical characteristics of a system. For this reason, it is important to clearly visualize the physical meaning and the course of changes in these characteristics due to the temperature change, the methods which they are experimentally determined by, and the limitations to which these changes are subject to [1-3]. The main thermophysical characteristics of materials that determine conditions for the heat treatment include enthalpy, heat capacity and coefficients of heat and temperature conductivity. Those parameters enter the thermal equation and determine the temperature field inside the substance. The thermophysical properties of the substance depend on a large number of factors, therefore the experiment is the only source for obtaining those characteristics [3]. However, the advent and development of a new direction, called the inverse heat conduction (IHC) problem, it became possible not only to research the form and content of simulation models

(SM) that reflect the phenomenological description of processes, but also a significant increase in the thermal experiment informativeness.

**Analysis of recent research and publications**

The problem relevance of developing numerical methods for solution of multidimensional systems of parabolic quasilinear equations describing the processes of heat and mass transfer can be considered as undeniable. One of the most interesting examples of such systems can be the equations of hydrodynamics and metallurgical thermophysics [4, 5]. Apparently, the mass solution of non-stationary problems of high accuracy order at the current level of technical capability and on the basis of traditional methods developed up to now seems to be possible only in the following circumstances.

First, the advent of new and inexpensive communication means of the computing technology stimulated development of new information technologies: structural programming, network operating systems, object-oriented programming, parallel information processing systems, etc. The parallel processing organization of information flows, the connection of parallelization problems with architecture of a PC, parallel programming systems, methods and algorithms of parallel computing are the key themes of the computer technology development at this stage [1, 6, 7].

Secondly, by now, certain trends have been emerged for development of computational methods with complex logical structure, which have a higher accuracy order comparing to the traditional finite difference methods [8 - 10]. Considerable progress in the solution of multidimensional spatial problems can be considered as a series of proposals that are not entirely equivalent to each other, yet which pursue one stereotypical goal to reduce the three-dimensional distribution problem of the variables change area to a sequence of schemes involving unknown quantities in only one direction, alternately in longitudinal, transverse, and vertical. A sufficiently detailed bibliography of these papers is presented in [8, 9]. It should be noted that the use of implicit schemes in this case leads to systems of linear algebraic equations (SLAEs) with a three-diagonal structure [9]. Thus, the adoption, as a methodological basis, of difference schemes of splitting, firstly, ensures an economical and stable implementation of numerical models by scalar sweep method. And, secondly, it is known that the greatest effect of a

parallel processor can be achieved when it is applied to perform matrix calculations of a linear algebra.

In this paper, the identification of heat conduction processes is considered on the equations solution example of the heat conductivity in the Cartesian coordinate system for the area of $y \in [y_o, yL]$, $t \in [0, \infty)$. Obviously, for given input data, this problem solution is simply realized by finite difference methods. Using the implicit timing schemes and the central differences in the spatial variable, we obtain a system of linear algebraic equations (SLAE) of a three-diagonal structure. Using the sweep method, we construct an economical difference scheme for solving a direct problem. From this algebraic SM analysis, it follows that for the grid area of the sought-for function definition $y_p, p = 1, 2, 3, \ldots, 2m, m \in Z$ in each $y_p - th$ grid node, the coefficients of SLAE include discrete values $\lambda_{p,1}, C\nu_{p,1}$. As can be seen, the number of unknowns $\lambda_{p,1}, C\nu_{p,1}$ is twice the number of grid equations. Such an unlocked SLAE, with known temperature values in the mesh nodes along a spatial variable, can have an infinite set of solutions with respect to unknowns $\lambda_{p,1}, C\nu_{p,1}$. Hence, a purely formal approach does not allow us to formulate a solution of IHC coefficient in the considered formulation.

**Statement of the Problem Research.**

The research purpose is to derive the corresponding class of temperature and gradient simulation models for research of the materials' thermophysical properties by reverse methods. The main research purpose is that the SM processing procedure as those that are controlled by input parameters, reduce, on the residual principle basis, to an extreme formulation. This approach allows to develop effective algorithms for solving quotient problems on SM of arbitrary accuracy order with adaptation of time modes of a thermophysical experiment.

Hereafter, we shall assume that the one-dimensional formulation of the thermal conductivity problems is the basic of a computational SM where there should be constructed the effective IHC solutions and algorithms for experimental data processing for the material thermophysical characteristics determination.

**Formation and analysis of simulations models of materials thermo-physical properties definition**

The problem solution could be obtained if the desired temperature dependences $\lambda(T)$, $C_{\nu}(T)$ are localized in the quadrants in the form of piecewise constant dependencies on temperature, both on the spatial variable and on time, and as a SM, construct the temperature and gradient dependence. We show that for each such spatiotemporal quadrant, the closed solutions of the original differential problem are effectively constructed by the Cauchy problem solutions:

$$T_{p+\varepsilon_{X,1}}(\varepsilon_t,\varepsilon_y)=\sum_{n=0}^{\infty}\left\{\frac{\varepsilon_y^{2n}}{(2n)!}\frac{1}{a_p^n}\frac{d^nT_{p,1}(\varepsilon_t)}{d\varepsilon_t^n}-(\frac{1}{\lambda_p})\frac{\varepsilon_y^{2n+1}}{(2n+1)!}\frac{1}{a_p{}^n}\frac{d^nT_{p,2}(\varepsilon_t)}{d\varepsilon_t^n}\right\}, \quad (1)$$

where $p=\overline{1,2m-1}$ are the numbers of grid nodes in the spatial area $y\in[y_0,y_L]$; $T_{p,1}(\varepsilon_t)$, $T_{p,2}(\varepsilon_t)$ are the Cauchy data (temperature and flow) given at the nodes of the grid area with $\varepsilon_y=0$; $a_p$ is an unmatched grid coefficient of the temperature conductivity ($a_p=\frac{\lambda_{p,1}}{CV_{p,1}}\frac{Dt1}{Dy1^2}$). The spatial and temporal variables in (1) are normalized by the dependences:

$$\left.\begin{aligned}\varepsilon_y&=\frac{y-y_p}{y_{p+1}-y_p}\in[-1,1]\\ \varepsilon_t&=\frac{t-t_{j-1}}{t_j-t_{j-1}}\in[0,1]\end{aligned}\right\}. \quad (2)$$

For the p-th grid nodes distributed uniformly, the Cauchy problem solution allows constructing the closed simulation models of unknown Cauchy data in the form of a system of ordinary differential equations (SODE). Putting in (1) $\varepsilon_y=\pm1$ we obtain the SODE of the N-th order:

$$\left.\begin{aligned}\sum_{n=0}^{N}\frac{1/a_p^n}{(2n)!}T_{p,1}^{(n)}(\varepsilon_t)&=\frac{1}{2}(T_{p+1,1}(\varepsilon_t)+T_{p-1,1}(\varepsilon_t))\\ -\frac{1}{\lambda_p}\sum_{n=0}^{N}\frac{1/a_p^n}{(2n+1)!}T_{p,2}^{(n)}(\varepsilon_t)&=\frac{1}{2}(T_{p+1,1}(\varepsilon_t)-T_{p-1,1}(\varepsilon_t))\end{aligned}\right\},\ N\in Z, \quad (3)$$

continuous in the time area. For instance, with N = 1 we obtain a first-order SODE in the Cauchy form, where the right-hand sides are assumed

to be known functions of time. In this case, it is expedient to construct a solution in a piecewise analytical form:

$$\left.\begin{aligned} T_{p,1}(\varepsilon_t) &= T^*_{p,1}(\varepsilon_t) + (T_{p,1}(0) - T^*_{p,1}(0))\ell^{-2a_p\varepsilon_t} \\ T_{p,2}(\varepsilon_t) &= T^*_{p,2}(\varepsilon_t) + (T_{p,2}(0) - T^*_{p,2}(0))\ell^{-6a_p\xi_t} \end{aligned}\right\}, \quad (4)$$

where $\left\{T^*_{p,1}(\varepsilon_t), T^*_{p,2}(\varepsilon_t)\right\}$ are particular solutions of inhomogeneous equations, $\left\{T_{p,1}(\theta), T_{p,2}(\theta)\right\}$ are known initial data. In the more general case, for an arbitrary value of the integer parameter of N arrangement, it is expedient to proceed from the differential equations (3) to a normal first-order SODE with a Cauchy form. Thus, the partial differential equation integration is reduced to the first-order SODE integration in Cauchy form, which can be used to solve the coefficient problems as those that are controlled by the SM in relation to the coefficients of heat and temperature conductivity. It should also be emphasized that the inclusion of the integer N parameter in the SM as an input value allows constructing the SM with an arbitrary accuracy order and an approximate order adoption.

**The reduction of determination problem of materials' thermal-physical properties to extreme formulation**

One of the promising directions for processing heat transfer problems by reverse methods is to bring them to extreme formulations by numerical methods of optimization theory. In the exact extreme formulation, the definition of parameters $\lambda_{p,1}$ *and* $Cv_{p,1}$ on SM (3) or (4) will correspond to minimization of discrepancies in the form of functionals:

$$\left.\begin{aligned} J_{p,1}(R) &= (T_{p,1}(\varepsilon_t, R) - f(\varepsilon_t, R))^2 \\ J_{p,2}(R) &= (T_{p,2}(\varepsilon_t, R) - Q(\varepsilon_t, R))^2 \end{aligned}\right\}, \quad (5)$$

where R are the sought-for control parameters.

The $J_{p,1}, J_{p,2}$ values in space $L_2$ in such a formulation can be considered as functions of the variables R. Their numerical value determines the distance in the functional space $L_2$ between the given $f(\varepsilon_t, R)$ , $Q(\varepsilon_t, R)$ quantities known from the experiment and that are being modeled by $T_{p,1}(\varepsilon_t, R), T_{p,2}(\varepsilon_t, R)$ on the controlled SM (3,4).

In each concrete case, on the basis of a priori information, it is possible to describe with some certainty, a certain admissible set of in-

put parameters R. Then, if we regard the SM as controllable, then the control parameters should be selected so determine its minimum. In the vicinity of the minimum, the value of the functional can be represented by a Taylor series expansion:

$$J_{\upsilon+\varepsilon_9 1}(q) = J_{\nu,1} + \varepsilon_R J_{\nu,2} + \varepsilon_R^2 J_{\nu,3} + \ldots, \quad (6)$$

where $\varepsilon_q = \dfrac{R - R_\nu}{R_{\nu+1} - R_\nu}$ is the normalized argument of the function; $J_{\nu,2}$, $J_{\nu,3}$.... – are the Taylor's components of the first and second order.

Retaining in the expansion (6) three summands and using the central differences for the Taylor components $J_{\nu,2}$, $J_{\nu,3}$

$$\left.\begin{aligned} J_{\nu,2} &= \frac{1}{2}(J_{\nu+1,1} - J_{\nu-1,1}) \\ J_{\nu,3} &= \frac{1}{2}(J_{\nu+1,1} + J_{\nu-1,1} - 2J_{\nu,1}) \end{aligned}\right\}, \quad (7)$$

after taking the derivative and after equating its value to zero, it becomes possible to construct an interpolation formula:

$$R = R_\nu - (\frac{1}{2})(R_{\nu+1} - R_\nu)\frac{J_{\nu+1} - J_{\nu-1}}{J_{\nu+1} + J_{\nu-1} - 2J_\nu}, \quad (8)$$

which allows arranging an iteration cycle. From this algorithm it follows that once the separation segment of the sought-for control parameter $\{R_{\text{P}+1}, R_{\text{P}-1}\}$, is set, where the disparaty in the functional (5) changes sign, further refinement of the control parameter in solving IHC can be refined recursively by formula (8) with any preassigned accuracy.

**Experimental data and the processing**

An important stage of the research was to develop a package of applied programs (PAP) for the coefficient problems solution of heat conduction by methods of simulation modeling [10]. The package was created taking into account the requirements of object-oriented programming. The simulation procedure was based on application of a multiprocessor computing system [11]. The PAP is designed for processing thermophysical experiments by inverse methods. Its creation main purpose was to provide practical assistance to the researcher at all stages of experimental data processing.

In this section of the research, additional conditions are considered allowing to divide the researched problem into two: the tempera-

ture and flow. The first one allows solving the coefficient problems in the whole given range of temperature variation with the control parameter in the form of the thermal diffusivity coefficient (model 1), the other is in the form of thermal conductivity or heat capacity (model 2). This approach corresponds to the classical methods of technical thermophysics. The SM 1 and 2 research is carried out by the method of straight lines. Moreover, model 1 (for example, algebraic or functional) and model 2 (gradient) allow solving the coefficient problem in an extreme formulation. As a test problem, it was proposed to determine the thermophysical properties of a particular industrial material [3]. The properties of coke made from gas coal were researched. For this, the temperature field of a sample with the shape of a cylinder was simulated. When solving such a coefficient problem, the following initial data were used: the thermal diffusivity coefficient $a_0 = a$, $N = 5$. The results of simulation performed by means of a multiprocessor computing system are shown in Fig. 1. The solution of the coefficient problem was carried out with control over the dimensionless coefficient of thermal diffusivity with $R = a / a_0$. From the simulation results analysis (Fig. 1) it follows that the disparity minimum corresponds to the value of the parameter $R \approx 1$. The exact value of the control parameter $R = 1$. For the heat conduction problem from tabular data $\lambda = 0.16$. Such a parameter identification is shown in Fig. 2.

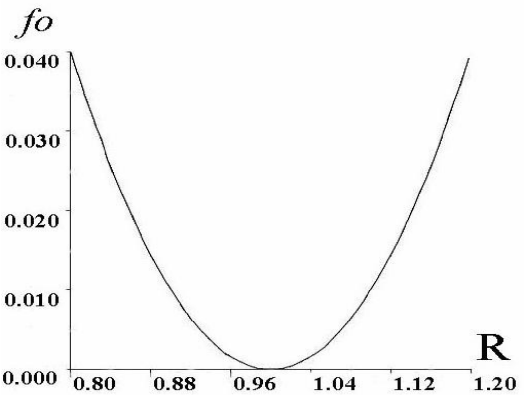


Fig. 1 - The computation results graph of the coefficient problem with $R = a / a_0$ the control parameter relative to the thermal diffusivity coefficient

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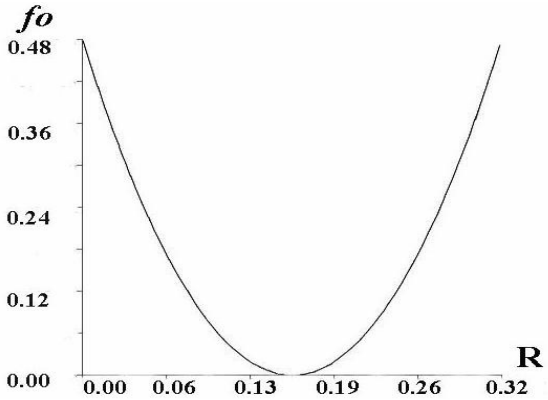


Fig. 2 - The computation results graph of the coefficient problem with $R = \lambda$ the control parameter relative to the thermal conductivity coefficient

The developed algorithm for solving the coefficient problem can be considered satisfactory, since its version using exact input data absolutely coincides with the exact result of the analytical solution, and the errors in the ccomputational results of the recovered causal characteristics, wherein included the input data error, approximately equal the output data error.

**Conclusions**

The solution of the inverse coefficient problem in the proposed formulation is reduced to a direct determination of the functionals values sequences (5) in simulation models (3) and the computation of the minimal carriers in them $J_{\min}$. The determination procedure of $J_{\min}$ can be implemented by simple sorting or by changing the sign $J^*(a) \cdot J^*(b)$ on the segment of R=a, R=b, where for the linear functional value (5) $(a < b)$. It is clear that $J^*(R) = 0$ a separated segment $R \in [a, b]$ has a root. The values refinement of this root can be realized with any preassigned accuracy in dependence (8) or, for example, by the chords or tangents method.

It should be noted that the partition of the total time interval into independent intervals with the solution of inverse problems in each of them according to the scheme indicated above allows determining the unknown parameters value as temperature functions $T_{p,1}(T)$. Therefore, the subsequent stage of processing experimental data is to construct the temperature dependences $\lambda_{p,1}(T), Cv(T)$ in the form of certain polynomial expansions of one degree or another by the method of mathematical planning and regression analysis. At this stage, to verify and establish

the adequacy, it is advisable to use a discrete nonlinear SM within a full space-time interval.

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