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METABK 59(1) 105-108 (2020)
UDC – UDK 669.011/53-536.7:621.78:658.562:517.1.086.5:621.3.036=111

METALLURGICAL THERMOPHYSICS PROCESSES IDENTIFICATION BASED ON EXTREME ALGORITHMS OF HIGH ORDER OF ACCURACY

Received – Primljeno: 2019-04-12
Accepted – Prihvaćeno: 2019-07-25
Preliminary Note – Prethodno priopćenje

The article is devoted the problem to researh the materials thermophysical properties by the inverse methods. Corresponding class of mathematical models is derived. The main research purpose is that the simulation models 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 simulation models of arbitrary accuracy order with adaptation of time modes of a thermophysical experiment. A package of applied problems had been developed for solving the coefficient problems of the heat-conductiving with the methods of mathematical simulation. Creation of package had been carried out considering the requirements of the object-oriented programming.

Keywords: metallurgical thermophysics, coefficient tasks, extreme algorithms, mathematical models, heat transfer.

INTRODUCTION

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 [1, 2].

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 personal computer (PC), parallel programming systems, methods and algorithms of parallel computing are the key themes of the computer technology development at this stage [3, 4].

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 [5,6].

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The main research purpose is that the simulation model (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.

FORMATION AND ANALYSIS OF SIMULATIONS MODELS OF MATERIALS THERMOPHYSICAL PROPERTIES DEFINITION

The problem solution could be obtained if the desired temperature dependences $\lambda(T)$, $Cv\ (T)$ 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:

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

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) $\varepsilon_y = \pm 1$; we obtain the SODE of the *N*-th order:

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

- 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:

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

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 input parameters *R*. Then, if we regard the SM as controllable, then the control parameters should be selected so that the functionals (5) are minimal. If the the acceptable range for changing control parameters are covered by *Rv*, grid nodes, then for their given values the functionals (5) can be calculated. Thus, the $\{J(Rv)\}$ sequence is minimizing if the limit allows to determine its minimum. In the vicinity of the minimum, the value of the functional can be represented by a Taylor series expansion:

$$J_{v+\varepsilon_9 1}(q) = J_{v,1} + \varepsilon_R J_{v,2} + \varepsilon_R^2 J_{v,3} + ..., \quad (6)$$

where $\varepsilon_q = \frac{R - R_v}{R_{v+1} - R_v}$ is the normalized argument of the function; $J_{v,2}, J_{v,3}$... – 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 $J_{v,2}, J_{v,3}$

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

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

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

which allows arranging an iteration cycle. From this algorithm it follows that once the separation segment of the sought-for control parameter $\{R_{P+1}, R_{P-2}\}$, 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 [6]. 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 [7]. 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 temperature 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 [8]. 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 Figure 1. The solution of the coefficient problem was carried out with control over the dimension-

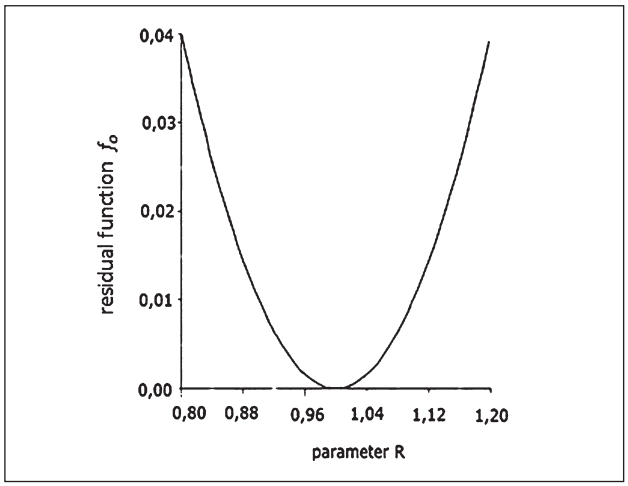

Figure 1 The computation results graph of the coefficient problem with $R = a / a_0$ the control parameter relative to the thermal diffusivity coefficient

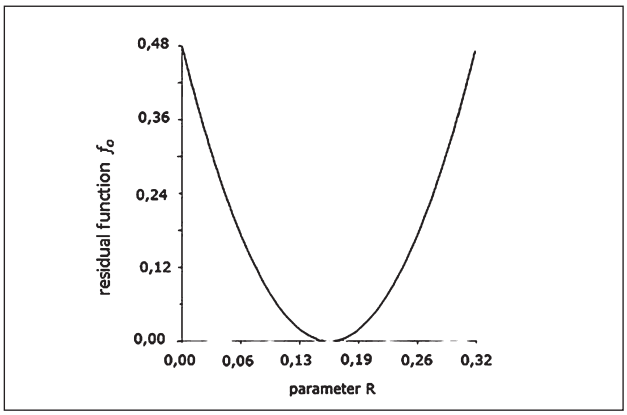

Figure 2 The computation results graph of the coefficient problem with R = λ the control parameter relative to the thermal conductivity coefficient

less coefficient of thermal diffusivity with $R = a / a_0$. From the simulation results analysis (Figure 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 Figure 2.

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.

CONCLUSION

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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Note: The responsible for English language is V.V. Busygin, Dnipro, Ukraine