and Lewis numbers; ρ, density; α, slope of liquidus line on state diagram; ν, μ, a, λ, k, D_2, c, k_0, ν_m, β_T, β_D, kinematic viscosity, dynamic viscosity, thermal diffusivity, thermal conductivity, permeability, diffusion coefficient, specific heat, impurity distribution coefficient, magnetic viscosity, and coefficients of thermal and concentrational volume expansion; g, acceleration due to gravity; θ_L, θ_S, θ_C T_C, liquidus, solidus, and crystallization temperatures; $k_* = 1 - k_0\rho_1/\rho_2$; $\langle U_2\rangle$, $\langle P_2\rangle$, $\langle\rho_2\rangle$, $\langle(j\times B)_2\rangle$, volume means of quantities in the liquid phase; $\langle U\rangle_2$ true volume mean velocity of liquid phase; L, latent heat of phase transition; $Da = k/x_0^2$, $Pr_m = \nu_m/\nu$ Darcy's number and magnetic Prandtl number; $Pr* = Pr_m/Pr$; S, electrovortex-flow parameter; v_r, v_z, r, z, φ, dimensionless radial and vertical velocity components and coordinates, electric potential; $Pr_e = Pr\nu_e/\nu$; $\langle V\rangle_2$ $\langle\omega\rangle$, $\langle\psi\rangle$ dimensionless true volume mean velocity, volume mean vortex velocity, and volume mean current function of the liquid phase; $\varphi_0 = \alpha C_0/T_2^0$; $K = L/(c_2T_2^0)$; $c_* = 1 + (c_1/c_2 - 1)\xi - K\partial\xi/\partial\Theta$; $\lambda = \lambda_1/\lambda_2 - 1$; $\rho_* = \rho_1/\rho_2 - 1$; q_J, q, dimensionless power of Joule heating and heat sinks in the pellet and the alloy; r_0, radius of ESM ingot; $\nu* = \nu*(\xi)$, effective kinematic viscosity [4]. Indices: 1, solid phase; 2, melt; 3) ingot mold (mold); 4) heat-insulation bushes.

LITERATURE CITED

1. R. I. Nigmatulin, Principles of Mechanics of Heterogeneous Media [in Russian], Moscow (1978).
2. V. T. Borisov, Theory of Two-Phase Zone of Metallic Casting [in Russian], Moscow (1987).
3. I. L. Povkh, F. V. Nedopekin, and V. V. Belousov, Dokl. Akad. Nauk UkrSSR, Ser. A, No. 9, 82-85 (1986).
4. F. V. Nedopekin and S. S. Petrenko, Insh. Fiz. Zh., 97, No. 2, 286-293 (1984).
5. F. V. Nedopekin and S. S. Petrenko, Teplofiz. Vys. Temp., 23, No. 3, 549-555 (1985).
6. F. V. Nedopekin and V. S. Borodin, Izv. Akad. Nauk SSSR, Met., No. 5, 216-222 (1987).
7. A. A. Samarskii, Theory of Difference Schemes [in Russian], Moscow (1977).
8. L. A. Kozdoba, Solution of Nonlinear Heat-Conduction Problems [in Russian], Kiev (1976).
9. I. L. Povkh, F. V. Nedopekin, and V. S. Borodin, Dokl. Akad. Nauk UkrSSR, Ser. A, No. 8, 38-40 (1985).
10. F. V. Nedopekin, S. S. Petrenko, V. F. Polyakov, and V. Ya, Minevich, Izv. Akad, Nauk SSSR, Met., No. 5, 64-69 (1985).
11. E. D. Taranov et al., Investigation of Hydrodynamic Processes in the Casting of Irregularly shaped Ingots [in Russian], Kiev (1984).
12. V. S. Borodin, V. M. Melikhov, F. V. Nedopekin, et al., Izv. Vyssh. Uchebn. Zaved., Chern. Met., No. 7, 72-76 (1987).

STRUCTURAL PARAMETRIC METHOD OF IDENTIFICATION OF MATHEMATICAL MODELS OF TECHNOLOGICAL PROCESSES

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UDC 536.24

A method is proposed for simultaneous estimation of the model parameters and their quality according to a set of criteria. Models of solidification in a chill mold are considered as an example.

The distinguishing singularity of any sufficiently complex technological process is the possibility of development of a whole series of competing models for its mathematical description, that could formally be represented in the form $Y = f(X, \Theta)$. In addition to the parameteric identification problems here, the estimate of Θ using models and test data, questions of structural identification, i.e., selection of the best model out of the available set, also occur.

As is mentioned in [1], these problems are interrelated since there is no sense in comparing models for accuracy prior to estimation of the parameters, and refining the parameters of a model of inadequate structure.

Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 57, No. 3, pp. 459-463, September, 1989. Original article submitted March 23, 1988.

0022-0841/89/5703-1080$12.50 © Plenum Publishing Corporation

Analysis of attempts at identification in a complex [2] shows that the main obstacles on the road to constructing a constructive method of estimating the model quality and the values of its parameters are the presence of several particular model quality criteria, there non-equivalence, the difficulty of formalizing particular criteria because of uncertainties associated with subjective preferences of the researcher and having a non-statistical nature in this connection. To overcome the difficulties mentioned the apparatus of the theory of odd sets [3] is utilized in this paper.

Rejecting such aspects as the exploitational characteristics of the model, in a first approximation it can be assumed that the collective estimate of its quality is determined by the criteria for accuracy of prediction and physicality of the parameter values. The physicality criterion is equivalent to the requirement that the estimated values of the adaptive parameters fall into a physically allowable range of their values. The boundaries of these latter are quite indistinct since they are ordinarily estimated on the basis of disconnected literature data. Moreover, different values of the parameter within the limits of the allowable range are often not equivalent from the viewpoint of the researcher. The desirability functions $\mu(\Theta)$ [3] that grow from 0 to 1 as Θ changes from the boundary of the allowable range to the domain of most preferable values, are used to formalized such criteria in the method being proposed.

Despite the known arbitrariness in assigning $\mu(\Theta)$, such criteria are more informative that the simple demand that Θ fall into a given domain.

Utilization of the desirability functions can also expand the informativity of the accuracy criteria. Thus, for instance, by using desirability functions $\mu(Y_c - Y_e)$ that are non-symmetric with respect to Y_e, the great preference of the exaggerated or lowered computed values can be taken into account. Let there be m accuracy criteria $\mu_{Y_i}(Y_i)$, $i = 1, \ldots, m$ dependent on the component of the vector of the model output variables Y_i and k physicality criteria $\mu_{\Theta_j}(\Theta_j)$, $j = 1, \ldots, k$, dependent on the components of the parameter vector Θ_j.

It is shown in [4] where different methods of convoluting particular criteria into a global criterion were investigated, that the optimal modification is the convolution proposed in [5]. Taking account of these results, the convolution of quality criteria for any point of an experiment X_i in which values of the input and output variables are known can be represented in the form

$$D(X_i, \Theta) = \min(\mu_{Y_1}^{\alpha_{Y_1}}(Y_1(X_i)), \ldots, \mu_{Y_m}^{\alpha_{Y_m}}(Y_m(X_i)), \mu_{\Theta_1}^{\alpha_{\Theta_1}}(\Theta_1), \ldots, \mu_{\Theta_k}^{\alpha_{\Theta_k}}(\Theta_k)), \tag{1}$$

where $\alpha_{y1}, \ldots, \alpha_{\Theta k}$ are coefficients of the relative importance of particular criteria. The method elucidated in [3], whose crux consists of the pairwise estimation of the relative significance of all the criteria, was utilized for their estimation. Each estimate is characterized by its numerical value entered in a square matrix of pairwise comparisons, whose number of rows and columns equal the number of criteria. The desired relative importance coefficients, or ranks, are found by the method in [3] by solving the eigenvalue problem for pairwise comparison matrices. The method being utilized for ranking the criteria permits solving a complex problem for estimating their significance in terms of a simpler pairwise comparison procedure.

Besides the accuracy and physicality criteria, (1) can include any others, for instance, the desirability function $\mu_\tau(\tau)$ determined by means of the machine time expenditure τ.

Taking into account that $\Theta_1, \ldots, \Theta_k$, can be variated within the limits of the allowable bands as well as that, as follows from (1), the maximal D correspond to the maximal values of the particular criteria, the estimate of the model quality at the points X_i is representable in the form

$$D_\Theta(X_i) = \max_\Theta D(X_i, \Theta). \tag{2}$$

Evaluating (2) in the whole set of points of the experiment $X_1, \ldots, X_N$, we obtain the set $D_{1\Theta}(X_1), \ldots, D_{N\Theta}(X_N)$. The hypothetical "ideal" model should evidently satisfy all the particular criteria completely. Taking account of (1) and (2), it follows from the normalization condition to one for these latter that $D_{\mathrm{i},i\Theta}(X_i) = 1$, should be satisfied for such a model at all points of the experiment, where $D_{i\Theta} \leqslant D_{\mathrm{i},i\Theta}$. Consequently $D_{i\Theta}$ can be considered as a measure of the nearness of the model to the hypothetical "ideal", which permits the formal introduction of the odd set DD = $(D_{i\Theta}/X_i)$, into the domain of the experiment, where $D_{i\Theta}$ can be interpreted as the value of a certain desirability function characterizing the degree of satisfaction of the requirement on the model at the points X_i.

Developed in [6] are methods of formalizing and later operating by using odd sets with objects of linguistic nature, including propositions in natural language. Using this methodology, the odd set DD can be given the following linguistic interpretation: "the model is adequate in the set of points of the experiment $X_1, \ldots, X_N$". Because $D_{i\Theta}\leqslant 1$, the assertion about adequacy is relative in nature.

By using the linguistic interpretation of the odd set DD a measure of model quality can be introduced that relies on the quantitative equivalent of the degree of definiteness (evenness) of the proposition about the adequacy of the model. To do this, a quantitative measure of evenness that is governed by the volume of the domain of intersection of the odd set and its complement [7], was used. In the case of odd sets this domain is nonempty and the broader it is the more the odd set differs from the even, and therefore, the higher the degree of its oddness. Modifying somewhat the evenness measure introduced in [7] in application to our conditions, it can strictly be shown that the quantitative measure of the definiteness of the proposition about the quality of the model is estimated by a simple expression.

$$D_m = \frac{1}{N} \sum_{i=1}^{N} D_{i\Theta}. \tag{3}$$

It is clear that upon comparison of a series of models the best will possess maximal D_m.

Under the real conditions of performing experiments it can turn out that the possibility of realizing each of them is characterized by the probability P_i, $i = 1, \ldots, N$. Experiments can be performed at different times with different accuracy and with a different degree of control on the influence of external effects. Analysis of these factors can result in the formation of desirability functions $\mu_x(X_i)$ that characterize the quality of the experiment.

In such cases D_m is evaluated by means of the generalized formula $D_m = \frac{1}{N}\sum_{i=1}^{N} P_i \min(\mu_x(X_i), D_{i\Theta})$.

The parameters are estimated by means of the formulas

$$\Theta_l = \sum_{i=1}^{N} \Theta_{il} D_{i\Theta} \Big/ \Big(\sum_{i=1}^{N} D_{i\Theta}\Big),\ l = 1, \ldots, k, \tag{4}$$

where $(\Theta_{1i}, \ldots, \Theta_{ki}) = \arg\max D(X_i, \Theta)$.

It is seen from (4) that within the framework of the method being proposed the parameters are estimated with suitability of the different points of the experiment being taken into account for identification of the models at these points in terms of the quality estimates, which, in sum, also permits designation of this method as structural-parametric.

The method being proposed has been used earlier to identify mathematical models of thermal and power processes during hot rolling of aluminum alloys [8]. The method is used in this paper for a comparative estimation of the quality of models of the solidification process. The experiments were performed for casting Al and Zn in a 140 mm high steel cylindrical heat insulated chill mold with a 97 mm inner radius and 15 mm wall thickness. The temperatures were measured at the center of the casting $T_1(\tau)$ and at a 1 mm depth from the chill mold working surface $T_2(\tau)$. At the time of removal of the overheating, i.e., at $T_1 = T_k$ the liquid residue was poured off and the thickness was measured of the frozen crust. By means of the measured values of $T_2(\tau)$ the heat flux, $q(\tau)$, on the working surface of the chill mold was restored by solving an inverse heat conduction problem in order to obtain the boundary conditions for formulating the problem of heat transfer during solidification.

Two competing mathematical models of the process were investigated. In the first (model 1), the extensively utilized method [9] permitting implicitly taking account of convective mixing in the liquid phase by introducing the effective heat conduction coefficient was used. Model 1 can be represented in the following form in a cylindrical coordinate system

$$\rho_1 C_1 \frac{\partial Q_1}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r}\left(\lambda_1 r \frac{\partial Q_1}{\partial r}\right), \quad \lambda_1 \frac{\partial Q_1}{\partial r}\bigg|_{r=R} = q(\tau), \tag{5}$$

$$\rho_2 C_2 \frac{\partial Q_2}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r}\left(\lambda_e r \frac{\partial Q_2}{\partial r}\right), \tag{6}$$

$$\frac{\partial Q_2}{\partial r}\bigg|_{r=0} = 0, \; Q_1\bigg|_{\tau=0} = Q_2\bigg|_{\tau=0} = Q_0, \quad Q_1\bigg|_{r=R-\zeta(\tau)} = Q_2\bigg|_{r=R-\zeta(\tau)} = T_k, \tag{7}$$

$$\frac{d\xi}{d\tau} = \frac{\lambda_2}{\rho_2 L} \frac{\partial Q_2}{\partial r}\bigg|_{r=R-\zeta(\tau)} - \frac{\lambda_1}{\rho_1 L} \frac{\partial Q_1}{\partial r}\bigg|_{r=R-\zeta(\tau)}, \tag{8}$$

where the thermophysical coefficients depend on the temperature and in conformity with [9] $\lambda_e = \lambda_0 + a(Q_2(0, \tau) - T_k)^n$. The model parameters a, n depend on the thermophysical and rheological characteristics of the process and require identification under specific conditions.

It was assumed in the construction of model 2 that there are no temperature gradients over the melt thickness in practice because of intense convective mixing, which permits considering Q_2 as the mean temperature of the liquid core. Consequently,

$$\frac{\partial Q_2}{\partial \tau} = -\frac{2\alpha(Q_2 - T_k)}{\rho_2 C_2 (R - \xi(\tau))}; \quad \frac{d\xi}{d\tau} = \\ = \frac{\lambda_1}{\rho_1 L} \frac{\partial Q_1}{\partial r}\bigg|_{r=R-\zeta(\tau)} - \frac{\alpha(Q_2 - T_k)}{\rho_1 L},$$

are introduced into model 2 in place of (6) and (8), where [9] $\alpha = b(Q_2 - T_k)^{n_1}$.

According to the theory, the model parameters n and n_1 are identical under identical casting conditions, while the parameters a and b differ by a factor. Numerical solutions were sought for both models by using the expanding mesh method. Estimates of the model accuracy were performed by the particular quality index

$$S_1 = \frac{1}{\tau_M}\left(\int_0^{\tau_M} (Q_2(0, \tau) - T_1(\tau))^2 d\tau\right)^{0,5}, \quad S_2 = \max_\tau |Q_2(0, \tau) - T_1(\tau)|,$$

$$S_3 = (\zeta(\tau_M) - H)/H, \quad S_4 = Q_2(0, \tau_M) - T_1(\tau_M).$$

Under these conditions the last quality index is of independent value since it characterizes the accuracy of predicting the time of total removal of the heating τ_m.

Preliminary numerical experiments for the variation of a, n, b and n_1 in physically allowable ranges permitted estimation of the maximal and minimal allowable errors. The information obtained was used to construct desirability functions of particular criteria that had the form $\mu_1 = 1 - S_1/40$, $\mu_2 = 1 - S_2/47$, say for S_1 and S_2. The functions $\mu_3(S_3)$ and $\mu_4(S_4)$ were represented by somewhat more complex nonsymmetric functions of their arguments. Because n and n_1 have an identical physical meaning, a common desirability function $\mu_5(n)$ constructed on the basis of the recommendations in [9] and the results of preliminary numerical experiments was used to describe the physicality criterion of their values.

No clear-cut preferences within the domains of their allowable values were disclosed successfully for the parameters a and b, consequently, no physicality criteria were introduced for them. Finally (2) was represented in the form

$$D_\Theta(X_i) = \max_{\Theta_1\Theta_2} \min (\mu_1^{\alpha_1}, \; \mu_2^{\alpha_2}, \; \mu_3^{\alpha_3}, \; \mu_4^{\alpha_4}, \; \mu_5^{\alpha_5}), \tag{9}$$

where Θ_1, Θ_2 — are the parameters a, n or b, n_1 depending on the selection of the model.

The matrix of pairwise criteria comparison was constructed with the great importance of the accuracy criteria taken into account, which yielded the summarizing estimate $\alpha_1 = 2.62$; $\alpha_2 = 0.98$; $\alpha_3 = 0.53$; $\alpha_4 = 0.53$; $\alpha_5 = 0.33$.

The maximin formulation results in multi-extremality and insufficient smoothness of the function (9). Consequently, the method of successive quadratic approximations [10], that has a number of advantages over classical methods under these conditions, was used in searching for the extremum.

For a series of tests with Al for models 1 and 2, respectively, $D_{m1} = 0.47$, $D_{m2} = 0.72$ were obtained by means of (3), and $D_{m1} = 0.78$, $D_{m2} = 0.73$ for tests with Zn.

It is hence seen that model 2 assures more stable and, on the average, more significant estimates of the quality criterion D_m of the models, which indicates its greater preferability.

Upon substitution of the parameters estimated by means of (4) in the model 2, the maximal errors hold for the prediction of the crust thickness and do not exceed 8% in the worst case.

The reason for the lesser adequacy of model 1, at first glance, evidently is the richer physical content as follows. Error compensation because of not taking account of convection in model 1 is realized by imposition of a certain perturbation by the introduction of λ_e. It is known that artificial methods of this kind work well although the perturbations are not large. In our case the latter is equivalent to the requirement $|\lambda_0 - \lambda_e|/\lambda_0 < 1$. However, as practice shows, the necessary model accuracy is achieved only for values of λ_e exceeding λ_0 many times [11]. It is clear that this carries model 1 too far away from reality and makes it non-physical.

The example considered permits an assessment of the constructivity of the proposed method, and its suitability for the solution of specific problems of structural-parametric identification.

NOTATION

X, Y, input and output variables of the model; Θ are model parameters; Y_c, Y_e, computed and experimental output variables; Q_1, Q_2, temperature fields in the solid and liquid phases; τ, r, time and radial coordinate, Q_0, temperature of the melt being cast; ρ_1, C_1, λ_1 solid phase density, specific heat, and thermal conductivity; ρ_2, C_2, λ_2, liquid phase density, specific heat, and heat conductivity; L, latent specific heat of melting; T_k, melting point; $\xi(\tau)$ running crust thickness; R, inner radius of the crystallizer; λ_0, heat conduction coefficient of the fixed melt; α, heat transfer coefficient between the melt and the solid phase, and τ_m, freezing time.

LITERATURE CITED

1. V. V. Nalimov and T. I. Golikov, Logical Foundations for Experiment Planning [in Russian], Moscow (1981).
2. L. S. Polak, ed. Application of Computational Mathematics in Chemical and Physical Kinetics [in Russian], Moscow (1969).
3. S. A. Orlovskii, Decision Making Problems For Fuzzy Original Information [in Russian], Moscow (1981).
4. P. V. Sevast'yanov, Control of Distributed Systems with Mobile Action [in Russian], Kuibyshev (1983), pp. 142-143.
5. R. R. Yager, Int. J. Man-Mach. Stud., 9, No. 4, 375-382 (1977).
6. L. Zadeh. Concept of the Linguistic Variable and Its Application to Approximate Decision Making [Russian translation], Moscow (1976).
7. R. R. Yager, Int. J. Gen. Syst., 5, No. 4, 221-229 (1979).
8. N. V. Diligenskii, P. V. Zevast'yanov, and N. V. Tumanov, Inzh. Fiz. Zh., 45, No. 5, 814-818 (1983).
9. G. F. Balandin, Principles of the Theory of Molding Castings [in Russian], Pt. 1, Moscow (1976).
10. N. V. Diligenskii, P. V. Sevast'yanov, and N. V. Tumanov, Methods and Facilities for Machine Diagnostics of Gas Turbine Engines [in Russian], Khar'kov (1980), pp. 18-19.
11. L. Shmrga, Solidification and Crystallization of Steel Ingots [in Russian], Moscow (1985).