A model at any of these levels should be open, i.e., the mathematical formalization should allow one to incorporate additional units that either describe different processes or else refine the couplings between elements. Also, the mathematical techniques and the logic of the couplings should provide, if necessary, for combining models at the different levels in application to any particular system.

NOTATION

T, temperature; **r**, spatial coordinate; n, normal; t, time; λ, thermal conductivity; ρ, density; c_p, specific heat; c_m, mass heat capacity of a lumped element; k_{ij}, conductivity between elements i and j of model; q_v, source function; q_{ext}, heat flux from the surroundings to the element; q_{co}, heat flux characterizing thermal interaction of elements; D_j, space region corresponding to element j of model; Γ_j, boundary of D_j; Γ_{ext} and Γ_{int}, sets of external and internal boundaries; N and N_α, numbers of distributed and lumped elements; subscripts: i, j, model element; α, lumped element.

CONCEPTUAL ALGORITHMS FOR ANALYSIS OF EXPERIMENTAL DATA

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A study is made of process simulation in inverse situations. Some problems arising in this approach are discussed, and a study is made of the choice of solution form, as well as of solution technique.

An important aspect of computer assistance in thermophysical research is to design algorithms for interpreting results; inverse treatments are often involved [1, 2]. In the treatment of experimental data, one often has to determine the causes of an observed effect, and inverse treatments provide a basis for analysis, which involves concepts in the interpretation of data. In practice, one often has the necessary information on the object in the form of models for conservation laws. Incorporation of a model into an analysis algorithm provides for more profound study of the structure and relevant factors. The corresponding algorithms may therefore be called conceptual, since the analysis is performed by inverse simulation. Simulation involves transfer from a general functional description to some particular description, which distinguishes this approach from other ways of solving inverse problems. In other words, conceptual algorithms presuppose the solution of more general problems, in which the formalization applies to the model and not to the initial data. The result is a model for an experiment that can provide characteristics of the process that are not accessible to direct observation, including the dynamic behavior of the object and so on.

We now consider ways of designing conceptual algorithms. We assume that we have chosen a model

$$L_a u = f, \tag{1}$$

and some observations are given

$$u^\delta = \bar{u} + \varepsilon$$

with a known value for the norm of the deviation from the true value:

$$\|u^\delta - \bar{u}\| \leqslant \delta. \tag{2}$$

In the choice of the model of (1) it is assumed that there exists a solution $u \in U$ that is unique in some metrical space U and that is continuously dependent on the initial data $a \in H$ and $f \in F$.

The model of (1) is the result of formalizing the process, so some of the parameters may be unknown or may differ from the actual object parameters. If appropriate a priori estimation is difficult, these parameters may be included in a vector a. Then the conceptual processing amounts to simultaneous determination of the state function $u \in U$ that satisfies the model throughout the relevant region of the independent variables together with the unknown parameters in metrical space H, which is the space of vector a. The latter requires additional information, where condition (2) is used.

In the construction of such a solution, it may happen that the result is not unique or that the solution is unstable. In the first case it is then necessary to establish a one-to-one correspondence between the desired quantities and the given

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sample, which enables one to recover the causes from the effect. In the second case, it becomes necessary to determine why the solution is not continuously dependent on the initial data. In such a case one should search for a method that can be applied to a broad class of inverse problems with varying levels and distributions for the errors of measurement, and which also allows one to convert from a general functional representation to a particular form. These specifications are met by regularization as described below.

We assume that the conditions for one-to-one correspondence are met and reduce the problem to

$$Sa = u^{\delta}, \tag{3}$$

where S is an operator that performs a mapping from H to U and which is specified inexplicitly by the form of model (1).

The errors of observation ϵ mean that the solution to (3) is unstable. Then the general theory of regularization [3] indicates that the solution must be sought in a space with a norm not weaker than the norm of the observation space. In practice, observations constitute a discrete set $u^{\delta} = \{u_{ij}^{\delta}\}_{i=\overline{1,n}}^{j=\overline{1,m}}$ at n points of measurement for each of the m points of observation. Such samples may correspond to a space with a Euclidean norm. Therefore a stable algorithm for solving (3) for real number spaces, when $H = E^p$, may be based on the following regularization:

$$\begin{gathered} \min_{a \in E^p} \max_{k \in [1,p]} |a_k|, \\ \sum_{j=1}^{n} (u_{ij}^{\delta} - u_{ij})^2 \leqslant \delta_i^2, \quad i = \overline{1, m}, \end{gathered} \tag{4}$$

where u is a function that satisfies model (1) with given a, i is the number of the observation point, and j is the instant of measurement.

Regularization can be performed as follows if another form is chosen for the error of measurement, e.g., the maximum deviation from the true value:

$$\begin{gathered} \min_{a \in E^p} \max_{k \in [1,p]} |a_k|, \\ \max_{j \in [1,n]} |u_{ij}^{\delta} - u_{ij}| \leqslant \delta_i, \quad i = \overline{1,m}. \end{gathered} \tag{5}$$

Therefore, conceptual analysis of models in which the unknown parameters are independent of the state function can be performed via the minimax problems of (4) or (5), in which one defines an element in the space of real numbers in conformity with the error of the input data. The criterion in (4) and (5) is the stabilizing functional

$$\Omega[a] = \max_{k} |a_k|,$$

and the δ_i denote the estimate of the error of measurement for element i in the observation set. Any change in the error estimator for a given set is reflected in the form of the coupling conditions, while the general mode of solution remains unchanged:

$$\begin{gathered} \min_{a \in H} \Omega[a], \\ \|u_i^{\delta} - u_i\| \leqslant \delta_i, \quad i = \overline{1,m}, \end{gathered} \tag{6}$$

where u_i is the value of the solution to (1) at the point of observation i and $\|\cdot\|$ is the norm corresponding to the form of the measurement-error estimator.

Other regularization schemes have been proposed [4, 5], but they differ in that the formulation of (6) is based on a particular use of the elements from the observation set u^{δ}, and a match is made to the error of the input data at each observation point separately, not via the overall dispersion. This reflects the form of observation common in practice. On the other hand, the formalization of (6) demonstrates a general approach to determination of the coefficients in the equation and to the conditions at the boundaries of the object.

This approach may be demonstrated in the solution of the following model problem. We assume that a physical process is described by the boundary-value problem

$$\frac{\partial \bar{u}}{\partial t} = \frac{1}{2} \frac{\partial^2 \bar{u}}{\partial x^2} + x + t - x^2, \quad x \in (0, 1), \; t \in (0, T), \tag{7}$$

$$\bar{u}|_{t=0} = x^2, \quad \bar{u}|_{x=0} = t, \quad \bar{u}|_{x=1} = 1 + t.$$

Simulation of the observed values for the state function is provided by specifying the quantities

$$u_{ij}^{\delta} = \bar{u}_{ij} + \varepsilon_{ij}, \quad i = \overline{1, m}, \quad j = \overline{1, n}, \tag{8}$$

for which we know the deviations

$$\delta_i^2 = \sum_{j=1}^{n} (u_{ij}^{\delta} - \bar{u}_{ij})_2, \quad i = \overline{1, m} \tag{9}$$

or

$$\delta_i = \max_{j \in [1,n]} |u_{ij}^{\delta} - \bar{u}_{ij}|, \quad i = \overline{1,m}, \tag{10}$$

where ϵ_{ij} are normally distributed random numbers of zero mathematical expectation. In practice, such estimators can be found by various means of statistical processing. A methodical study may be made of the numerical features of these algorithms by determining the δ_i from (9) and (10) in relation to the function

$$\bar{u} = t + xt + x^2 - x^2 t, \tag{11}$$

which is the exact solution to (7).

The resulting sample of the form of (8) will be analyzed by means of a four-parameter model as follows over the following observation parameters: m = 4, n = 10, and T = 1:

$$a_1 \frac{\partial u}{\partial t} = a_2 \frac{\partial^2 u}{\partial x^2} + a_3 \frac{\partial u}{\partial x} + a_4 u + x + t - x^2, \quad x \in (0, 1), \; t \in (0, T), \tag{12}$$

$$u|_{t=0} = x^2, \quad u|_{x=0} = t, \quad u|_{x=1} = 1 + t.$$

The choice of the model of (12) is not unique. One could use various other models that express the corresponding concepts. However, the same significant factors must always appear in the particular choice of model.

We do not propose to discuss in detail the uniqueness of the coefficients and merely note that one can demonstrate an unambiguous correspondence between the coefficients of (12) and the function of (11).

The solution to the problem of (12) with given values for the coefficients may be determined by a finite-difference method via a spatially centered Crank–Nicholson scheme. The penalty-function method enables one to reduce (4) and (5) to a problem in unconditional programming, in which a search is made coordinate by coordinate.

Table 1 represents results of identification of the model of (12) and shows that these regularization schemes can provide satisfactory solutions no matter whether the measurement dispersion is small or large. Further, scheme (5) gives a more accurate estimate of the model structure than does (4). Scheme (4) provides poor accuracy in the identification if the noise dispersion is large. In that case, a comparison can be made of the temperature discrepancies arising from the errors of measurement, and it is found that the solution has poor consistency in the observations, with the discrepancies much larger than the corresponding δ_i. We therefore consider the formulation

$$\min_{a \in E^p} \max_{k \in [1,p]} |a_k|,$$

$$\sum_{j=1}^{n} (u_{ij}^{\delta} - u_{ij})^2 = \delta_i^2, \quad i = \overline{1, m},$$

which provides improved accuracy.

One can specify the errors approximately in terms of the upper limit

$$\delta = \max_{i,j} |u_{ij}^{\delta} - \bar{u}_{ij}|$$

but this involves deterioration in the identification accuracy. In that case the spread in the errors in the observation set around the mean value is important. For noise dispersions $\sigma^2 = 10^{-4}$, one can simulate a single measurement, whereas five-fold measurements are required for $\sigma^2 = 10^{-2}$.

TABLE 1. Solution Results

Noise dispersion	Regularization scheme	Error estimator δ	Result for vector a
σ=0,01	(4)	0,0015; 0,00115; 0,00105; 0,00109	0,986; 0,464; 0,111; —0,093
	(5)	0,0353; 0,0151; 0,0197; 0,0153	0,992; 0,483; 0,061; —0,018
	(5)*	0,0353; 0,0353; 0,0353; 0,0353	0,381; 0,346; —0,459; —0,124
σ=0,1	(4)	0,0222; 0,0122; 0,0057; 0,0166	0,506; 0,447; —0,442; —0,105
	(5)	0,0996; 0,0888; 0,0418; 0,0706	0,984; 0,446; 0,113; —0,091
	(5)*	0,0996; 0,0996; 0,0996; 0,0996	0,791; 0,378; —0,239; 0,0756

*The upper limit of the error is specified.

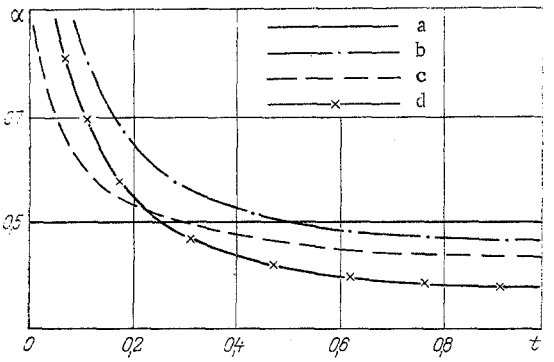

Fig. 1. Values of the heat-transfer coefficient: a) exact value; b, c) formulations of (4) and (5) respectively; and d) least squares.

These regularization schemes were compared on a sample u^δ with dispersion $\sigma^2 = 10^{-4}$, with least-squares processing. The resulting vector was a = (0.806; 0.375; 0.017; –0.235) and the accuracy in identifying the model of (7) was worse than that in regularization.

We now consider some applications of the simulation results. We perform a prediction starting from t = T and extending up to t = 10T for the dynamic behavior of an object identified from sample u^δ with dispersion $\sigma^2 = 10^{-4}$; in that case, the maximum deviation of the predicted state from the true state in (4) and (5) and in the least-squares method was, respectively, 0.1271, 0.1047, and 0.1285, which constituted 0.98, 0.79, and 1.04% of the value of $\bar{u}$ in each case.

This solution to the inverse problem also allows one to solve the common practical problem of estimating the heat-transfer coefficient from temperature measurements. Figure 1 shows values for this coefficient derived from

$$\alpha = a_2 \frac{\left.\dfrac{\partial u}{\partial x}\right|_{x=0}}{u|_{x=0} - u_{am}|_{x=0}},$$

where $u_{am}|_{x=0} = 0$ is a known temperature.

Therefore, the program package for the simulation involving inverse treatments can provide general models for experiments; in particular, it is possible to construct analysis algorithms that reflect the details of the process. The results show that common forms of error estimator (including unsmooth ones) can be used. These can improve the evaluation of the model structure. This approach may prove efficient and fruitful in research on complex processes.

NOTATION

L_a, model; a, unknown parameter vector; u, function describing process; u^δ, observed values; $\bar{u}$, true state; ϵ, measurement error; δ, norm of uncertainty; f, effect; U, H, F, metric spaces; T, upper limit of measurement; u_{am}, ambient temperature.

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A METHOD OF PROCESSING THE READINGS OF A GRAPHITE CALORIMETER

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A quasi-solution method has been applied to a nonlinear inverse problem in thermal conduction to process test data for a graphite calorimeter in a plasma jet.

Inverse problems in thermal conduction occur in experimental aerodynamics, particularly for heat transfer to models in wind tunnels, e.g., in relation to the testing of thermal shields and high-temperature constructional materials. These inverse problems have to be considered when it is necessary to calculate the temperature pattern in a model while the parameters of the external flow and the boundary conditions are not well established, e.g., in measurements on the nonstationary heat transfer from a high-temperature jet. A graphite calorimeter is used for the purpose here.

The calorimeter (Fig. 1) is a cylindrical graphite vessel having a flat bottom, into which is screwed a sensitive element of thickness 0.017 m and diameter 0.04 m. There are three Chromel–Alumel thermocouples of thickness 8×10^{-5} m inserted in the sensitive element near the center on the inside. The thermocouples are attached by contact welding to a layer of zirconium of thickness 10^{-4} m melted onto the graphite in a vacuum furnace.

The solution of the inverse problem for the graphite is complicated because the parameters are very much dependent on temperature, so the treatment is nonlinear. A stable solution is found by the quasisolution method [1-3]. One has to determine the heat-flux density from the temperature variation at the internal surface, which involves a nonlinear problem in thermal conduction for a one-dimensional wall in the following formulation: one is given a parametric compact family K of functions $q(\tau)$, from which one selects a time function for the heat flux $q_w(\tau)$ such that the theoretical time function for the temperature $T_t(\tau)$ at the internal surface of the wall corresponds best with the measured result $T_m(\tau)$, i.e., $q_w(\tau)$ is defined by the condition

$$\max_{0\leqslant\tau\leqslant\tau_{max}} |Aq_w(\tau) - T_m(\tau)| = \inf_K \max_{0\leqslant\tau\leqslant\tau_{max}} |Aq(\tau) - T_m(\tau)|,$$

where A is the finite-difference operator for the direct nonlinear thermal-conduction problem:

$$Aq(\tau) = T_t(\tau), \quad 0 \leqslant \tau < \tau_{max}.$$

The uniformly bounded and equally continuous parametric families of functions are compact in the space of continuous functions with a uniform-approximation metric. The heating conditions are close to those of regular modes, so the compact set is taken as a two-parameter family of exponential functions:

$$K \equiv \{q(\tau) : q(\tau) = Q\exp(-m\tau), \quad Q_{min}\leqslant Q\leqslant Q_{max}, \quad m_{min}\leqslant m\leqslant m_{max}\}.$$

The choice of the set in this form is justified by the good agreement between the theoretical result $T_t(\tau)$ and the measured one $T_m(\tau)$ (Fig. 2).

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