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ANALYSIS OF UNCERTAINTIES IN DYNAMIC THERMOPHYSICAL MEASUREMENTS

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A technique of analyzing the dependence of the uncertainty of results as applied to a thermophysical experiment is presented. The dependence of the uncertainty of the result of investigation of a sample under a temperature change on the number, uncertainty, and place and moment of experimental sampling is investigated. A comparative analysis of several approaches to solution of this problem is given.

In the last two decades, the NIST [1], under the aegis of the ISO [2], has proposed that the notion of uncertainty be used as the main means of expressing a measurement result. In Russia, the notion of uncertainty has not yet been used in normative documents, but the advantage of this innovation is being increasingly recognized [3]. In this paper, representing a continuation of [4–6], we show that this notion can be used in practice to good advantage, especially in the case where the uncertainty is presented in interval form. We will restrict our consideration to the case where, knowing the uncertainty of the measured quantities, it is necessary to estimate exactly the uncertainty of the result of an indirect measuring experiment. Such important problems as the efficiency and stability of the procedure of identification of the estimated parameters, the quality of the model of the measuring cell, and the systematic errors and their interpretation from the viewpoint of the uncertainty presented in interval form require an individual consideration.

Approaches Used and Their Essence. The initial information for determining the thermophysical parameters of an object of investigation is provided by the model of behavior of the measuring cell $T((q, \rho, xyz, t), (a, \lambda, c, \varepsilon))$ describing a change in the temperature field with time and in space and the experimental data $\{([q], [\rho], [xyz], [t], [T])\}$. The purpose of a thermophysical experiment is to estimate $[\alpha, \lambda, c, \varepsilon]$. The technique of analyzing the uncertainty of this estimation represents a series of procedures meant for determining the functional dependence $\Delta[a, \lambda, c, \varepsilon] = f\{([q], [\rho], [xyz], [t], [T])\}$; the uncertainty investigated depends on both the uncertainty of the data and their absolute values.

Of the four thermophysical parameters, only two can be independent. As the latter, λ and c are usually used. There are many variants of the division of model parameters into parameters measured directly in a working experiment, parameters determined in a calibration experiment, and parameters fixed in the process of designing of an experimental setup. To separate the significant characteristics of the approaches under consideration and take into account their important features we will act in the following way. The essence of the approaches will be described with the use of the maximum abstract model $T(p, m) = \{d\} \to [p]$, where p, m, and d are the parameters whose values are estimated, are fixed *a priori*, and are measured in the experiment considered respectively. The features of the methods will be considered in detail in the process of analysis of the example presented below.

Approach 1 (traditional). This method is the usual one; therefore, we will describe it only schematically without formalization and discussion of details, the great number of possible variants, and references. The information contained in the data is divided into two blocks: the "pure" measured data d and their uncertainty Δd. The problem of identification is easily solved in the case where there is a strictly necessary amount of data or in the case where there is a significant excess of data.

If the amount of data is smaller than the amount necessary for identification of the value of a model parameter, the problem does not have a reasonable solution at all.

If the amount of data is just enough for a single identification of the value of a parameter, its estimate obtained is taken as the solution p. We are to calculate the uncertainty of the result. In practice, calculations are carried

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out only in the first approximation on the basis of the sensitivity of the model to the change in the measured parameter $[p] = p \pm \Delta d \frac{\partial p}{\partial d}$. Taking into account more subtle effects caused by the nonlinearity of the sensitivity or the unequal accuracy of the data, if done, requires much greater expenses than the identification itself.

If the amount of data is just exceeded but still insufficient for regression analysis, its excess is difficult to efficiently use. These data are suitable at most to throw away the outliers (which usually represent the extreme values) and resort to the previous variant.

In the case of a large amount of data, one can use L^p statistics, in particular, the least-squares method. Although this method is not the best variant, it is commonly usual and simple and, what is more important, is legalized by many normative documents. The problem is that, as a result of its use, a valid estimate of the result, containing the estimate of the error, is obtained at once. The problem of compatibility of this estimate with the estimate obtained by the uncertainty of the data arises. There are no justified proposals on the solution of this problem. One of these estimates, the lower as a rule, is usually ignored. Of course, the uncertainty boundaries cannot be determined exactly in this case. It is common practice to assume that the estimate of a parameter and the estimate of its error are equally exact.

The method is not illustrative and involves a large number of assumptions, the admissibility of which is difficult or even impossible to verify in each individual experiment. A strong side of this method is its validity.

In the case where the data are in excess, an inverse variant of the least-squares method can be used. The essence of this variant is that a large number of the already obtained inverse solutions of the identification problem $\{p\}$ are used. Each solution is obtained by combining a necessary number of data samples. A large number of such combinations and, consequently, solutions can be obtained if there is an excess of data. The least-squares method is applied in a much more simple form only to the already obtained solutions. The excessively large dispersion of the obtained solutions, observed in practice, hinders the application of this approach.

Approach 2 ("jack-knife" method). The "jack-knife" methods represent relatively new developing statistical methods of analysis of data [7, 8]. There is a large number of varieties of these methods and many methods that are similar to them in ideas but with different names. The main idea is that the samples must be multiplied if their number is insufficient. These methods differ in the way in which this can be done and the way in which the samples obtained can be used. We will consider only the simplest variant following naturally from the structure of the data.

From n different elements of the data $[d]$ a scalar vector $\{d\}_n$, such that $d \in [d]$, is selected. One scalar value of the vector of the parameter p is identified by this set. The selection is repeated many times. A certain "cloud" of solutions $\{p\}$ is formed.

One uses very different methods of selection of the components of the vector $\{d\}_n$ both inside $[d]$ and from the set $\{[d]\}$: from orderly scanning algorithms of different types to a random selection by complex combinatorial laws, and different combinations of them. It is evident that two d cannot be selected from one $[d]$. It is clear that one can seek to use all $[d]$ and simultaneously distribute the samples from $\{[d]\}$ as uniformly as possible. It is also obvious that any desired number of estimates of the parameter sought can be obtained in this way. Problems do not usually arise at this stage.

Problems arise in the process of analysis of the cloud of solutions obtained in the space of parameters. It is clear that the cloud-density distribution contains information on both the values of the parameters sought and their uncertainty. The inclusion of the entire cloud into the solution is unreasonable, to say the least. It is usually divided with respect to the density and the included fraction of solutions. Substantiation of the selection criterion is a very difficult problem which does not yet have a satisfactory and simultaneously universal solution. For this reason, the method has not found wide application. The routine approach assumes that the obtained field of estimates has the properties of a random representation of the same quantity. Then the problem is solved by standard statistical means oriented to a fairly large sampling.

Approach 3 (interval method). The interval method reflects the essence of our proposal. This method is not statistical; conversely, it is purely deterministic. The method is based on the quite reasonable assumption that since a measuring experiment can be successful only in the case where $\exists p : T(p) \in [d]$, then $[p] = [\{\forall p\}] : T(p) \in \forall [d]$. In words this means that the estimation of the parameters sought (in interval form) includes only the values of the parameters for which the prediction of the model falls within practically all the obtained (interval) estimates of the experimental data.

An important feature of this approach is that the boundaries of the intervals are of particular significance. All the properties of the solution are determined first of all by the boundaries. The uncertainty can be large, but the boundaries can be determined very exactly in this case. The properties of the interval method are considered in more detail in [4–6].

Approach 4 (Bayes method). The essence of this method is that, under certain assumptions, the conditional probability of interest to us can be changed to the product of the densities of the probabilities. In our case, it is necessary to determine the probability of the event $P(p \mid T(p, t) \in \{d\})$, i.e., it is necessary to know the probability that the model correctly predicts the experimental results for the parameter p. The coordinates of the maximum of this probability are interpreted as the estimate of the experimental result, and the region where the probability has any significant value is interpreted as the uncertainty of this result. If it is assumed that the data samples are independent and the interfaces and errors are stationary, the following expression holds:

$$P\left(p \mid T(p) \in \{d\}\right) = \frac{P_{\mathrm{a}}(p) \prod_{i=1}^{N} P_i(d_i - T(p))}{\int_{\infty}^{N} P_{\mathrm{a}}(p) \prod_{i=1} P_i(d_i - T(p))\, dp},$$

where P_{a} is *a priori* information on the solution and P_i is the distribution of the probability of the ith element of the data.

The method makes it possible to take into account the individual statistics of each data sample P_i. Otherwise this is the usual statistical method. The proposed interpretation of the Bayes rule has been devised by us; therefore, we do not refer to a literature source. Nonetheless, the rules and properties of the method proposed correspond to other interpretations of the Bayes rule [9, 10].

Example. By way of example, let us consider the pulse method of measuring the thermophysical parameters. For the sake of definiteness, we will use the variant of a linear pulsed source in an unbounded medium. For invariable thermophysical parameters the temperature field is described by the expression

$$T(t, (\lambda, c), (x, q, \rho)) = \frac{q}{4\pi\lambda c\rho t} \exp\left(-\frac{\sqrt{c\rho}\, r^2}{4\sqrt{\lambda}\, t}\right).$$

In this example, we investigate only the dynamics of temperature propagation, assuming that the distance from the heater to the thermometer r as well as the density of the heat flux q and the density ρ of the material studied are exactly known. So as not to relate the model to a concrete class of materials, we normalize it in the following way. The thermal conductivity and the heat capacity each are normalized to the range [1, 2], the temperature change is normalized to the range [0, 1], and the time of the experiment is normalized to the range [0, 1] so that the temperature decreases to half the maximum value by the end of the experiment. In what follows, all the numerals are given in relative units. Finally we investigate the normalized model of the measuring experiment

$$T(t, (\lambda, c)) = \frac{A}{\lambda c t} \exp\left(-B\sqrt{\frac{c}{\lambda}}\,\frac{1}{t}\right), \tag{1}$$

where $A = q/(4\pi\rho) = 0.488$ and $B = \sqrt{\rho}\, r^2/4 = 0.18$. It is remarkable that for this model there is an analytical solution of the identification problem $((t_1, T_1), (t_2, T_2)) \to (\lambda, c)$

$$\lambda = \frac{B(t_1 - t_2)}{T_1 t_1} \frac{\sqrt{AT_1 t_1 \exp\left(-\ln\left(\frac{T_1 t_1}{T_2 t_2}\right)\frac{t_2}{t_1 - t_2}\right)}}{t_1 t_2 \ln\left(\frac{T_1 t_1}{T_2 t_2}\right)}, \quad c = \frac{t_2 \ln\left(\frac{T_1 t_1}{T_2 t_2}\right)}{BT_1(t_1 - t_2)} \sqrt{AT_1 t_1 \exp\left(-\ln\left(\frac{T_1 t_1}{T_2 t_2}\right)\frac{t_2}{t_1 - t_2}\right)}. \tag{2}$$

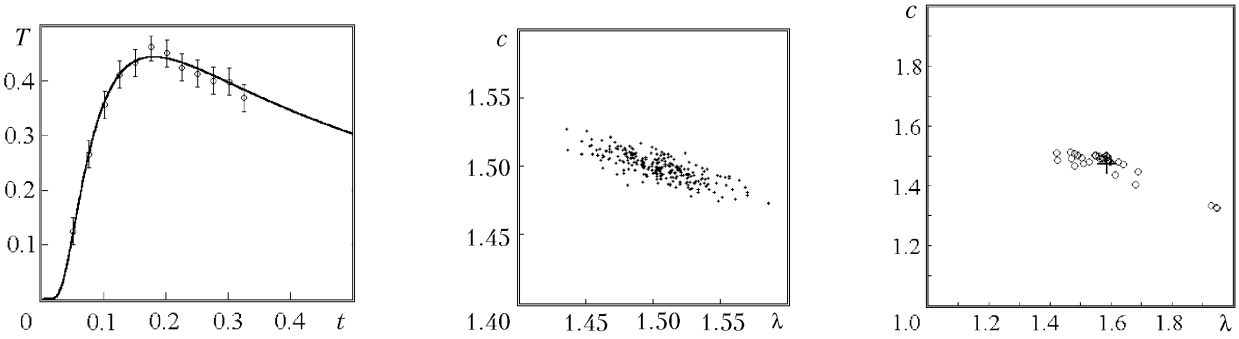

Fig. 1. Example of initial data against the background of the "true" solution.

Fig. 2. Result of a numerical experiment for repetition, 200 repetitions.

Fig. 3. Result of application of the inverted least-squares method when four nearest samples are ignored and 36 combinations of data samples out of 66 possible combinations are used. The obtained estimate of the measured parameters is denoted as +.

Data for the numerical experiment will be obtained in the following way. We will use $N = 12$ samples. For each t_i we calculate the temperature from (1) for the values of the parameters (1.5, 1.5) and distort the result obtained by the random normally distributed numbers with a dispersion of $\sigma = 0.0083$. It is assumed for simplicity that the confidence interval adheres to the law 3σ. The obtained distorted numbers in combination with their confidence interval will be considered as data similar to those shown in Fig. 1. We note that only the information on the temperature is uncertain; the information on the sampling time is left to be ideal. This significantly simplifies the representation of the results. Their real values and generality are impaired only slightly.

The direct least-squares method gives the result $(\lambda, c) = (1.541, 1.489)$ for these data. The calculation of the uncertainty by the deviation gives ± 0.087, by the uncertainty of the data gives ± 0.048, and by the deviation with a correction for the sensitivity to the parameters gives $(\pm 0.116, \pm 0.03)$. A more objective estimate of the uncertainty can be obtained from a numerical experiment by the principle of repetition. For this purpose, the above-described numerical experiment was repeated many times and the overall dimensions of the obtained "cloud" of solutions were estimated (Fig. 2).

We have obtained the following estimate of the dispersion: $[1.435, 1.586] = 1.504 \pm 0.075$, $[1.473, 1.528] = 1.499 \pm 0.027$. It is remarkable that the dispersion cloud is shaped as an ellipse, the slope of which is very difficult to calculate by the least-squares method. More exactly, the complexity of such a calculation exceeds the possibilities of the method.

The inverted least-squares method gives the results $(1.586 \pm 0.124,\ 1.473 \pm 0.049)$ (Fig. 3). The uncertainty has been calculated by the standard method from the dispersion $\{(\lambda, c)\}$. The main contribution to the estimate of the dispersion is made by the distant results. They in turn are obtained with the use of data samples closely spaced in time. Ignoring these data initially improves the result both in the accuracy of its estimation and in the estimation of the uncertainty. When the number of ignored neighborhoods increases, the estimation of the measured parameters initially improves but then, on the contrary, deteriorates because of the decrease in the total number of data taken into account. It is very difficult to calculate *a priori* the optimum number of ignored neighborhoods.

The jack-knife method has been implemented with the use of the inverse solution (2) (Fig. 4). From each of the 12 data samples (in interval form), we select 5000 scalar samples once again. A solution is obtained for each pair of the newly obtained samples. The traces of the data samples in the form of arcs are seen in the picture. The traces of the samples positioned on the rise and fall of the time dependence of the temperature differ very markedly. The traces of some pairs of samples merge together.

Although there is no general technique of obtaining the solution, the evident heuristic technique can be used in this concrete case. The uncertainty region covers the overlap that is constructed in the following way. The first line connects the closest points of the boundary arcs. The second line is approximately perpendicular to the first line and

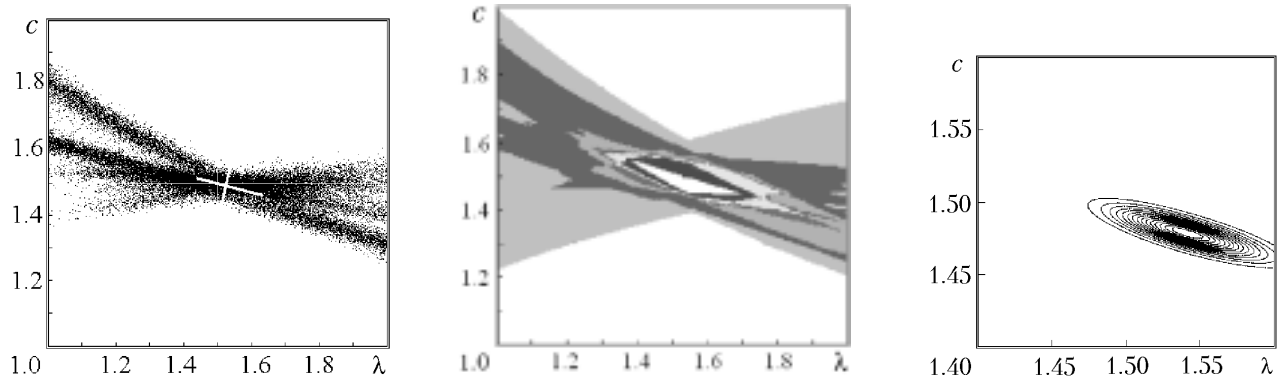

Fig. 4. Result of application of the jack-knife method in the case of repeated (5000 times) sampling from each data sample.

Fig. 5. Result of application of the interval method.

Fig. 6. Result of application of the Bayes method. The probability maximum is 0.002.

continues from the branching of the bands to another nearest branching. We have obtained the result (1.54 $\pm$ 0.09, 1.49 $\pm$ 0.06).

The use of the interval method makes it possible to completely transform the entire information contained in the data into a result in a very illustrative form (Fig. 5). The traces of each data sample are clearly seen in the form of individual bands in the picture (Fig. 5). The result is determined as the intersection of all these bands. The solution appears as an islet at the center of the picture. The result has both a dimension and a shape. It is most simply described in the form of dimensional intervals. In the example, we have obtained [(1.375, 1.72], [1.445, 1.545] = (1.547 $\pm$ 0.172. 1.495 $\pm$ 0.05).

A significant feature of the approach is the exceptional importance of the data boundaries for obtaining the boundaries of the solution. It is easy to show that the "true" result will be inside the uncertainty cross section if and only if the "true" value of the temperature lies inside all the data samples. Furthermore, a certain boundary of a certain data sample can be related to each boundary of the result if necessary. In actual fact, only these measurements (which form the solution) give useful information.

If there is reason to have doubts about a concrete data sample, it can easily be verified whether this sample makes a contribution to the estimation of the result. If the sample makes a contribution, it is excluded and another sample becomes responsible for the new boundary. The information on this subject is already contained in Fig. 5. Moreover, if we are doubtful of the correctness of the data and believe that at least one sample is incorrect, we can become reassured and select a figure of a lower level of uncertainty for the solution, for example, the figure that corresponds to $N-1$ coincidences of the prediction and the data.

The situation differs greatly from the situation that arises when the other considered approaches are used. The kind of probability law of dispersion of the values of the data is of no significance. This information can be obtained from more thorough processing of the experimental data. No a priori assumptions of the properties of the model and the features of the data are required at all. In this case, the information contained in the experimental data is not averaged and is not lost. All this makes it possible to use the interval approach as a basis for algorithms of fine processing of experimental data.

The Bayes method was used under the following assumptions. A priori information is the same probability of any value of the solution for the entire region of admissible values. The Gaussian probability density is true for each data sample with a center at the distorted point of the data. Now, to obtain the solution, it is necessary to obtain a prediction of the model for each combination of parameters which is of interest to us. Based on these predictions, the probabilities are calculated for each data sample and then they are multiplied together. Normalization of the probabilities was not used.

The result of application of the Bayes method is not so illustrative as the interval approach. An ideal two-dimensional Gaussian surface is obtained in each case. It is shown in the form of level lines in Fig. 6. The dimension

of the ellipse varies but insignificantly. The probability changes in a wide range (10^4–0.4). We have obtained the result (1.535 $\pm$ 0.07, 1.485 $\pm$ 0.02).

All the methods considered are approximately equivalent in relation to algorithmic simplicity. The same can be said about the calculation efficiency. As for the visibility of the results, the interval method offers an advantage over the other methods. This makes it possible to use it as a basis for more detailed processing of the experimental information. Its main advantage is the possibility of transmission of all the information contained in the data to the result. The Bayes method may also be of interest but only in the case where its application is the final point of the investigation.

NOTATION

a, thermal diffusivity; *c*, coefficient of heat capacity; *d*, element of abstract data; *q*, heat energy (density); *p*, abstract parameter; *r*, distance; *T*, temperature; *t*, time; *xyz*, geometric coordinates; ε, thermal activity, $\Delta[\bullet] = \bullet_{max} - \bullet_{min}$, uncertainty of the variable "•"; λ, thermal-conductivity coefficient; ρ, density of the material; [•], interval representation of the variable "•."

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