Optimal experiment design to estimate the thermal destruction parameters of materials

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Abstract. Results are presented in the work on mathematical modeling with respect to a simultaneous determining of the emissivity and thermal effect of sublimation for thermal insulating material as functions of temperature. Optimal experiment design based on influence of the external heat fluxes and some other parameters to the accuracy of the considered inverse problems solution has been studied.

1. Introduction
Mathematical modeling of processes of thermal interaction of destructive thermal insulating materials with high enthalpy gas flows should be based, in general, on solving the coupled problems of unsteady heat and mass transfer. Problems of this class are formulated in the form of a system of equations covered the whole complex of interconnected processes: the gas flow in the considered domain; the heat and mass transfer in the high-temperature boundary layer in the presence of chemical reactions in multi-component gas; surface destruction and heat transfer within the material.

Solution of the conjugated heat and mass transfer problems in the general formulation is a complex problem, and it is difficult to solve it at present. Therefore, it is necessary to generate simplified mathematical models, which covered approximately the complex processes under consideration. Approximate mathematical models usually contain a number of effective characteristics, each of which covered a certain set of individual phenomena and processes. In studying the interaction of materials with high-enthalpy gas flows it is necessary to determine some properties of materials characterized this interaction and included in heat balance equation on the external surface of considered specimens.

Direct measurement of the greater number of parameters of mathematical model of heat transfer is often impossible, and theoretical estimates are not accurate enough or even contradictory. Hence, a problem appears on how to determine parameters of heat transfer processes on the surface of the body through available experimental data processing. A method analyzed in this paper for determining unknown heat transfer characteristics is based on the iterative regularization of inverse problems, which at present are widely and successfully used in studying the internal heat transfer processes [1]. This method makes it possible to develop effective algorithms for determining unknown heat transfer parameters through the results of temperatures measurements.

In this paper we analyze the inverse problem of estimating the characteristics of surface thermal interaction of a destructed material with a high enthalpy gas flow. Here we assume that the heat-transfer process within the material is described by the heat conduction equation, one-dimensional in a space coordinate, with coefficients that are functions of temperature. In addition, it is assumed that the
destruction and removal of material occurs only in the gas phase. With these assumptions in particular case we can considered emissivity $\varepsilon(T)$ and the thermal effect of sublimation $\Delta Q_w(T)$ as the determined coefficients of the approximate mathematical model of the process of heat and mass transfer occurring in a certain time interval $[0, \tau_m]$ in the gas-solid system.

Consider a slab of thickness $b(\tau)$, the heat transfer in which is covered by a nonlinear heat-conduction equation. It is assumed that at the left boundary of the slab a boundary condition of the second kind is specified, while at the right of the slab the interaction with gas flow is assumed. The mathematical model of the process can be presented as

$$C(T)\frac{dT}{d\tau} = \frac{d}{dx}\left(\lambda(T)\frac{dT}{dx}\right)$$

$$T = T(x, \tau), \quad x \in (0, b), \quad \tau \in (0, \tau_m]$$

$$T(x, 0) = T_0(x), \quad x \in [0, b]$$

$$-\lambda(T(0, \tau))\frac{dT}{dx}(0, \tau) = q_r(\tau), \quad \tau \in (0, \tau_m]$$

$$-\lambda(T_w)\frac{dT_w}{dx} = q_w(\tau), \quad T_w = T(b, \tau), \quad \tau \in (0, \tau_m]$$

$$q_{3w}(\tau) = q_0(\tau) + e(T_w)\sigma T_w + G_w\Delta Q_w(T_w), \quad \tau \in (0, \tau_m]$$

The functions $\varepsilon(T)$ and $\Delta Q_w(T)$ are unknown. In addition, some experimental measurement of the temperature on the time are specified at some internal points of the slab with the coordinates $x_i$, $i = 1, M, M \geq 1$

$$T_{\exp}(x, \tau, \tau) = f_m(\tau), m = 1, M, \quad \tau \in (0, \tau_m]$$

### 2. Inverse problem

The inverse problem consists in determining the functions $\varepsilon(T)$, $\Delta Q_w(T)$ and $T(x, \tau)$, $x \in [a, b], \tau \in [0, \tau_m]$. It is evident that the problem of recovering the two functions $\varepsilon(T)$ and $\Delta Q_w(T)$ from the single equation (5) does not have a unique solution. Avoid the nonuniqueness, one must bring in additional data. A natural choice for this additional information is to use the data of some set of $N$ thermal experiments conducted on identical specimens but in different thermal disintegration regimes, under the hypothesis that in the different experiments the unknown characteristics have the same relationships. Here it is necessary that the number of different regimes should be at least no less than the number of unknown characteristics. With this approach one can provide a number of algebraic equations of the type of (5) equal to the number of desired characteristics, or even an excess of experimental information [2].

Proceeding from the principle of iterative regularization [1], the unknown function can be determined through minimization of discrepancy functional, when the unknown function is determined by gradient methods of the first order prior to a fulfillment of the condition

$$J(\varepsilon(T), \Delta Q_w(T)) = \sum_{n=1}^{N} \sum_{m=1}^{M} \sum_{t=0}^{\tau_n} \int \left(T(x_m, \tau) - f_m(t)\right)^2 dt \equiv \delta^2$$

where $T(x, \tau)$ is the temperature calculated using the model (1)-(5) with fixed values of $\varepsilon(T)$ and $\Delta Q_w(T)$; $\delta^2 = \sum_{n=1}^{N} \sum_{i=m}^{M} \int \sigma^2(x_m, \tau) dt \tau$ is the integral error of the temperature measurements; $\sigma^2(x_m, \tau)$ is the dispersion of the error in measuring the temperatures. If the desired function
depends on the temperature, parameterization of the unknown parameters is used in the following form. Suppose then that the unknown characteristics are given in their parametric form. With this purpose introduce in the interval \([T_{\min}, T_{\max}]\), two uniform difference grids with the number of nodes \(N_i, i=1,2\).

\[
\omega_i = \left\{ T_k = T_{\min} + (k-1)\Delta T, \quad k = 1, \frac{N_i-1}{2} \right\} \quad i = 1,2
\]

(8)

Approximating the unknown functions on these grids using the splines is

\[
e(T) = \sum_{k=1}^{N_e} e_k \varphi^e_k(T).
\]

\[
\Delta Q_w(T) = \sum_{k=1}^{N_Q} Q_k \varphi^Q_k(T).
\]

where \(\varphi^e_k(T), \quad k = 1, N_e\) and \(\varphi^Q_k(T), \quad k = 1, N_Q\) are the above mentioned systems of basic functions. As a result of approximation, the inverse problem is reduced to the search of a vector of unknown parameters \(\bar{p} = [p]^N_p\) in the Euclidean space \(E^N_p\) [1], with dimensions \(N_p = N_e + N_Q\).

To construct an iterative algorithm of the inverse problem solving a conjugate gradient method was used. Such a problem was considered in [3,4].

3. Optimal experiment design

As has been said above, the developed method of determining the \(e(T)\) and \(\Delta Q_w(T)\) of a material necessitates the solution of an ill-posed inverse problem. The accuracy of estimating of the desired properties is determined largely by the experimental merits, and one is connected with the problem of optimal experiment design. When the processing of the experimental data is the solution of ill-posed problems, optimal experiment design essentially entails the sampling of merits that will ensure the best conditioning of the computational algorithm [1,2,5]. The available a priori information about the experimental data are used to formulate a certain scalar criterion of optimality \(\Phi(\xi)\), which depends on the experiment design \(\xi\) and characterizes the conditioning of the algorithm for solving the inverse problem. It is reasonable to assume that \(\Phi(\xi)\) has a lower bound on the set of possible designs \(\Sigma\) and that optimal design \(\xi^*\) exists such that

\[
\xi^* = \arg \inf_{\xi \in \Sigma} \Phi(\xi)
\]

(11)

In order to formulate the experiment design problem, it is necessary to select the design criterion \(\Phi(\xi)\), to identify the experimental merits comprised in its actual design, i.e., the merits that significantly influence the criterion \(\Phi(\xi)\), and to formulate the domain of possible designs \(\Sigma\).

It has been shown [3] that the inverse problem of determining the thermal and radiative properties on the surface of a material can be considered as superpositioning of two problems: 1) the boundary inverse heat conduction problem of determining the heat flux \(q_i(\tau)\) into the specimen and the surface temperature \(T_w(\tau)\); 2) the problem of estimating the unknown material thermal and radiative properties from the heat balance equation at the external surface boundary. The influence of the number and coordinates of the thermosensors on the solution of the first problem has been studied in detail in [1,5]. The results show that a nonstationary measurement of the temperature at one internal point of the specimen is sufficient for reconstructing the heat flux \(q_i(\tau)\). As the number of sensors is increased, the convergence of the algorithm and the accuracy of the solution are improved at first, but only up to a point. The thermosensors must be placed as close as possible to the exposed surface. The solution of the second problem is not directly affected by the positions and number of the thermosensors (only via the accuracy of IHCP problem solution).
We analyze the influence of the external heat flux \( q_0(\tau) \) on the accuracy of solution of the given inverse problem by parametric variation of the heat flux. The following formula was used for simulation of the variation of the external heat flux:

\[
q_0(\tau) = K_q \tilde{q}_0(\tau), \quad K_q \in [0.5; 1.5]
\]

where \( \tilde{q}_0(\tau) \) is a certain specified function. The numerical simulation is carried out with the same input data and for solving the inverse problem as in [4]. The coefficient \( K_q \) is varied discretely with step equal to 0.1. For each value of \( K_q \) the error of reconstruction of the functions \( \varepsilon(T) \) and \( \Delta Q_w(T) \) are calculated as

\[
\delta_\varepsilon = \left[ \int_{T_{\text{min}}}^{T_{\text{max}}} (\varepsilon(T) - \tilde{\varepsilon}(T))^2 dT \right]^{1/2}
\]

\[
\delta_Q = \left[ \int_{T_{\text{min}}}^{T_{\text{max}}} (\Delta Q_w(T) - \tilde{\Delta Q}_w(T))^2 dT \right]^{1/2}
\]

where \( \tilde{\varepsilon}(T) \) and \( \tilde{\Delta Q}_w(T) \) are the a priori specified (or exact) temperature dependences of the emissivity and thermal effect of sublimation, \( \varepsilon(T) \) and \( \Delta Q_w(T) \) are the functions reconstructed from the solution of inverse problem, \( T_{\text{min}} \) and \( T_{\text{max}} \) are the minimum and maximum temperatures of the exposed surface. The results of the calculations are shown in Fig. 1 and evince the significant influence of the nature of the external heat flux on the accuracy of solution of the inverse problem.

Figure 1. Influence of the experimental merits on the accuracy of solution of the inverse problem. a- heat flux \( q_0 \); b - duration of experiment \( \tau \); c - specimen thickness \( b \). 1 - \( \delta_\varepsilon \), 2 - \( \delta_Q \), 3 - optimal criterion \( (\det A \times 10^{-32}) \) as a function of experimental merits.
The dependence of the accuracy of solution of the inverse problem on the duration of the experiment

\[ \tilde{\tau}_m = K_\varepsilon \tau_m, \quad K_\varepsilon \in [0.5;1.5], \quad \tau_m = 30 \text{ sec} \]  

(14)
is studied similarly. To preclude, insofar as possible, the influence of the external heat flux, its variation is transformed to the form

\[ q_0(\tau) = \tilde{q}_0(K_\varepsilon \tau) \]  

(15)

which enables us to impart a similar behavior to the thermal state of the specimen. The formula governing the influence of the initial slab thickness are following

\[ b = K_b b, \quad K_b \in [0.5;1.5] \]  

(16)
The results of a parametric analysis of the accuracy of solution of the inverse problem are also shown in Figure 1. On the basis of the above simulation the following set of merits is used in the present paper for the experiment design

\[ \xi = \{b, \tau_m, q_0(\tau)\} \]  

(17)

where \( b \in R, \quad \tau_m \in R, \quad q_0(\tau) \in C^0 \) and \( \xi \in \Sigma R \times R \times C^0 \). In order to solve the problem (11), it is necessary to determine the domain of possible designs \( \Sigma \). The following considerations must be taken into account in forming this set:

1) \( b \in [b_l, b_u] \);
2) \( \tau_m \in [\Delta \tau_m, \tau_m^*] \);
3) \( \alpha_0(\tau) \leq q_0 \leq \beta_0(\tau), \quad \alpha_1(\tau) \leq q_0 \leq \beta_0(\tau) \).

Following [3] the determination of the vector \( \bar{p} = \{p\}_{l}^{N_l} \) can be reduced to the solution of the system of linear equations

\[ A \bar{p} = d \]  

(18)

where (without number of experiments)

\[ A = \{a_{km}\}, \quad k = 1, N, \quad m = 1, N, \]  

\[ a_{km} = \int_{0}^{\tau_m} \sigma^2 T_w^{0} \varphi_k^{0}(T_w) \varphi_k^{0}(T_m) d\tau, \quad k \leq N_e, m \leq N_e, \]  

\[ a_{km} = \int_{0}^{\tau_m} G_w \varphi_k^{0}(T_w) \varphi_k^{0}(T_w) d\tau, \quad k > N_e, m > N_e, \]  

\[ a_{km} = \int_{0}^{\tau_m} \sigma T_w^{4} G_w \varphi_k^{0}(T_w) \varphi_k^{0}(T_w) d\tau, \quad \text{for other cases}. \]

The heat flux \( q_\lambda \) into the specimen and the surface temperature \( T_w \) can be regarded as input data for problem (18), and \( A \) is the Fisher information matrix of the considered system [6,7]. Following [7], the determinant of \( A \) is adopted as the optimality criterion of the experimental design:

\[ \Phi(\xi) = -\det A(\xi) \]  

(19)

Problem (11) then acquires the form

\[ \xi^* = \arg \inf_{\xi \in \Sigma} (-\det A(\xi)), \quad \Sigma \in R \times R \times C^0 \]  

(20)
Figure 1 shows the results of mathematical modeling, which demonstrate the high sensitivity of the values of the criterion (19) to variations of the experimental merits and its good compatibilities with the error of inverse problem solution.

The optimal design problem (20) is solved by the numerical projective gradient method of optimization. The iterative process is formulated as follows in this case:

1) an initial approximation of the experiment design \( \xi^0 \) is specified, e.g., in the form \( \xi^0 = \{b_2, \Delta r_m^s, \beta_0 \} \);

2) the value of the gradient of the functional \( \Phi_{s'} (\xi) \), the descent step \( \alpha^s \), and the experimental design in the next iteration are computed, where

\[
\xi^{s+1} = \xi^s + \alpha^s \left( \Phi_{s'} (\xi) \right)^t, \quad s = 0, 1, 2, ..., \xi \in \Sigma
\]

\[
\xi^{s+1} = \{b^{s+1}, \Delta r_m^{s+1}, q_0^{s+1} (r), \tau \in \left[ 0; \tau_m^{s+1} \right] \}
\]

\[
\Phi_{s'} (\xi) = \left[ (\Phi_{s'} (\xi))^t; (\Phi_{s'} (\xi))^t; (\Phi_{s'} (\xi))^t \right]
\]

(21)

3) the iterative process is stopped when the optimality criterion has the same value in two successive iterations, i.e., when the following condition is satisfied

\[
\left| \left| \Phi_{s+1} (\xi) - \Phi_{s} (\xi) \right| \right| < \epsilon^s
\]

(22)

where \( \epsilon^s > 0 \) is the a priori specified relative error of exit from the iterative process.

The size of the step \( \alpha^s \) is selected on the basis of the condition

\[
\min_{\alpha' \in R, \xi \in \Sigma} \Phi \left( \xi^s + \alpha^s \left( \Phi_{s'} (\xi) \right)^t \right)
\]

(23)

by one of the conventional techniques of one-dimensional optimization.

### 4. Numerical simulation

The above-described procedure for experiment design of the conditions of a nonstationary experiment has been implemented in the form of a computer code. For the practical application of the proposed procedure, an experiment to determine the emissivity and thermal effect of sublimation of thermal insulated materials [4] is analyzed. The thermal and radiative properties of the material are taken from [4]. The optimal experimental merits are chosen in application to a radiative test facility, in which time variation of the heat flux to the specimen is created by variation of the electric power in the heater. The constraints of variation of experiment design parameters are given in Table 1. The lower constraint is used as initial values for the thickness, the average values is used as initial values for the duration of the experiment, and the initial flux to the specimen is varied linearly from zero to the maximum possible value with maximum rate.

The functions given in [4] is taken as the a priori information about the function \( \epsilon(T) \) and \( \Delta Q_w(T) \). The inner surface of the sample is assumed to be thermally insulated. The intermediate values of the experimental merits in the third and tenth iterations during the iterative solving of the experiment design problem are shown in Table 2 and Figure 2. Iterative process is presented in Figure 3. As a practical demonstration of the effectiveness of the selected optimality criterion, we have solved the inverse problem of reconstructing the emissivity \( \epsilon(T) \) and \( \Delta Q_w(T) \) for the experimental merits obtained in each iteration of the solution of the experiment design problem, and we have determined the error of the solution presented in Figure 4.
5. Conclusions
The results show that the optimal experiment designs have a very complex nature for different materials of the class in question. This fact suggests that the values obtained for the slab thickness, the duration of the experiment, and the heat flux to the material should be recommended for practical work in the experimental investigation of the $e(T)$ and $\Delta Q_w(T)$ of some classes of materials using definite experimental facilities with characteristics close to those indicated above. The extension of the numerical results of the present study to other classes of materials and experimental equipment, and other heat transfer processes on the inner surface of the specimens requires additional studies, because the physical quantities governing the indicated factors are used directly in the mathematical model (1) – (6) and can have a significant influence on the optimal experiment design.

Since estimating the emissivity and thermal effect of sublimation are part of the problem of complete identification of the heat-transfer model (it is equations (1) – (5) in the given case) the accuracy in determining $e(T)$ and $\Delta Q_w(T)$ corresponds to the errors in the preliminarily derived characteristics of $C, \lambda$, etc., in view of the identity of the methods applied.

Note also that the results of the nonsteady experiment may be analyzed to determine the internal thermophysical characteristics ($C, \lambda$) as well as the emissivity and thermal effect of sublimation.

| Table 1 Constraints | Table 2. Some results of the optimal experiment design problem |
|---------------------|-------------------------------------------------------------|
| Parameters          | Parameters                                                  | Iteration number. |
| 0.04 $b_1, m$       | 0.04 $b_1, m$                                               | 0              |
| 0.04 $b_2, m$       | 0.04 $b_2, m$                                               | 0.0485         |
| 10 $\tau_{m1}, \text{sec}$ | 20 $\tau_{m1}, \text{sec}$ | 29.3          |
| 10 $\tau_{m2}, \text{sec}$ | 20 $\tau_{m2}, \text{sec}$ | 30.4          |

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Figure 2 Heat flux (two experiments) as a parameter of experiment design. 1 – constraints, 2 - zeros iteration, 3 third iteration, 4 tenth iteration
Figure 3. Iterative process. 1 –optimal criterion (det $A \times 10^{-32}$) as a function of iteration number $s$, 2 - $\delta_x$, 3 - $\delta_Q$.

Figure 4. Results of emissivity (a) and thermal effect of sublimation estimating. 1 - exact values, 2 – result of the simulation of inverse problems solving with experimental merits from zeros iteration of experiment design, 3 - from third iteration, 4 – from tenth iteration.

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