On the Determination of the Volumetric Heat Capacity and the Thermal Conductivity of a Substance in the Three-Dimensional Case

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In the creation of new materials, a situation occurs when the volumetric heat capacity and the thermal conductivity of substance depend only on temperature and this dependences are unknown.

In this context, the problem arises of determining the temperature dependence of the volumetric heat capacity and thermal conductivity from experimental observations of temperature field dynamics.

A similar problem arises when a complex thermal process is described by a simplified mathematical model. An example is the mathematical simulation of heat transfer in complex porous composite materials, where a noticeable role is played by radiation heat transfer.

Formulation of the Problem

$$C(T(s,t)\frac{\partial T(s,t)}{\partial t} = div_s\Big(K\big(T(s,t)\big)\cdot \nabla_s T(s,t)\Big), \qquad (s,t) \in \{Q \times (0,\Theta)\}, \qquad (1)$$

$$T(s,0) = w_0(s), \qquad s \in \bar{Q}, \qquad (2)$$

$$T(s,t) = w_{\partial Q}(s,t), \qquad s \in \partial Q,\ \ 0 \le t \le \Theta. \qquad (3)$$

Consider the sample of substance that has the shape of a right parallelepiped of length $\boldsymbol{X}$, width $\boldsymbol{Y}$, and height $\boldsymbol{Z}$.

$x \in [0, X]$, $y \in [0, Y]$, $z \in [0, Z]$ – the Cartesian coordinate of the point $s = (x, y, z)$;
$t \in [0, \Theta]$ – the time;
$Q = \{\ (0, X) \times (0, Y) \times (0, Z)\ \}$;
$T(s,t)$ – the temperature at the point s at the time t;
$C(T)$ – the volumetric heat capacity of the material;
$K(T)$ – the thermal conductivity;
$w_0(s)$, $w_{\partial Q}(s,t)$ – given functions.

The Cost Functional 1 :

$$\Phi\big(C(T), K(T)\big) = \int_0^{\Theta} \int_Q \mu(s,t) \cdot [T(s,t) - Y(s,t)]^2 ds\, dt,$$

$\mu(s,t) \geq 0$ – given parameter;
$Y(s,t)$ – given experimental temperature field.

The optimal control problem is to find the optimal control $\{C(T), K(T)\}$ **and the corresponding optimal solution** $T(s,t)$ **to the problem (1-3) that minimizes functional** $\Phi(C(T), K(T))$.

The optimal control problem always has more than one solution:

$\{C^*(T), K^*(T)\}$ – **solution** $\rightarrow$ $\{\lambda C^*(T), \lambda K^*(T)\}$ – **solution.**

Additional condition: for example, $\chi(T) = \frac{C(T)}{K(T)}$.

Optimal Control Problem in the Discrete Case

1). The **desired functions** $C(T)$ and $K(T)$, $T \in [a,b]$ were approximated by continuous piecewise linear functions.

2). The **domain** $G = \{(s,t):\ Q \times (0 < t < \Theta)\}$ was broken up by grid planes $\{x_n\}_{n=0}^{N}$, $\{y_i\}_{i=0}^{I}$, $\{z_l\}_{l=0}^{L}$ and $\left\{\tilde{t}^j\right\}_{j=0}^{J}$ into a series of parallelepipeds. In each of the resulting parallelepipeds, the law of thermal balance must be met. The result is a finite difference scheme that approximates the mixed problem (1)-(3).

3). To solve the **direct problem**, the iterative version of locally one-dimensional scheme was used.

$x -$ direction:

$$\frac{V_{nil} \cdot C(T_{nil}^{j+1/3}) \cdot (T_{nil}^{j+1/3} - T_{nil}^{j})}{\tau^j/3} =$$

$$= \frac{\left(K(T_{n+1,il}^{j+1/3}) + K(T_{nil}^{j+1/3})\right)}{2} \cdot \frac{\left(T_{n+1,il}^{j+1/3} - T_{nil}^{j+1/3}\right)}{h_n^x} \cdot S_{il}^{yz} -$$

$$- \frac{\left(K(T_{nil}^{j+1/3}) + K(T_{n-1,il}^{j+1/3})\right)}{2} \cdot \frac{\left(T_{nil}^{j+1/3} - T_{n-1,il}^{j+1/3}\right)}{h_{n-1}^x} \cdot S_{il}^{yz};$$

$y-$direction:

$$\frac{V_{nil}\cdot C(T_{nil}^{j+2/3})\cdot(T_{nil}^{j+2/3}-T_{nil}^{j+1/3})}{\tau^j/3}=$$

$$=\frac{\left(K(T_{n,i+1,l}^{j+2/3})+K(T_{nil}^{j+2/3})\right)}{2}\cdot\frac{\left(T_{n,i+1,l}^{j+2/3}-T_{nil}^{j+2/3}\right)}{h_i^y}\cdot S_{nl}^{xz}-$$

$$-\frac{\left(K(T_{nil}^{j+2/3})+K(T_{n,i-1,l}^{j+2/3})\right)}{2}\cdot\frac{\left(T_{nil}^{j+2/3}-T_{n,i-1,l}^{j+2/3}\right)}{h_{i-1}^y}\cdot S_{nl}^{xz};$$

$z-$direction:

$$\frac{V_{nil}\cdot C(T_{nil}^{j+1})\cdot(T_{nil}^{j+1}-T_{nil}^{j+2/3})}{\tau^j/3}=$$

$$=\frac{\left(K(T_{ni,l+1}^{j+1})+K(T_{nil}^{j+1})\right)}{2}\cdot\frac{\left(T_{ni,l+1}^{j+1}-T_{nil}^{j+1}\right)}{h_l^z}\cdot S_{ni}^{xy}-$$

$$-\frac{\left(K(T_{nil}^{j+1})+K(T_{ni,l-1}^{j+1})\right)}{2}\cdot\frac{\left(T_{nil}^{j+1}-T_{ni,l-1}^{j+1}\right)}{h_{l-1}^z}\cdot S_{ni}^{xy};$$

$$(n=\overline{1,N-1},\quad i=\overline{1,I-1},\quad l=\overline{1,L-1},\quad j=\overline{0,J-1}).$$

$S_{il}^{yz}, S_{nl}^{xz}, S_{ni}^{xy}$ - areas of the faces of the calculation cell, V_{nil} - the volume of this cell.

4). The **Cost functional** approximation:

$$\Phi(K(T), C(T)) \cong F(k_0, k_1, \ldots, k_M, c_0, c_1, \ldots, c_M) =$$

$$= \sum_{j=1}^{J} \sum_{l=1}^{L-1} \sum_{i=1}^{I-1} \sum_{n=1}^{N-1} \left((T_{nil}^{j} - Y_{nil}^{j})^2 \cdot \mu_{nil}^{j} h_n^x h_i^y h_l^z \tau^j \right).$$

5). The **Optimal Control Problem** was solved numerically by gradient method. It is known that when using gradient methods, it is extremely important to determine the exact values of gradients. The gradient of the Cost function was calculated with the help of Fast Automatic Differentiation technique.

Fast Automatic Differentiation Technique

Let we have a continuously differentiable scalar function (Cost function)

$$W(z,u), \quad where\ z = z(u)$$

Let we have a continuously differentiable vector function (Phase constraints)

$$\overline{\Phi}(z,u) = \overline{0}_n$$

The function $\Omega(u) = W(z(u),u)$ **is a complex function**

(Function of Control)

Idea: Lagrange multiplier method

The calculation of complex function may be represented as some multi-step process:

$$z_i = F(i, Z_i, U_i), \quad 1 \le i \le n \qquad (1)$$

Z_i – is the set of all components of z_j, that are on the right - hand side of (1)

U_i – is the set of all components of u_j, that are on the right - hand side of (1)

Then the gradient of a complex function $\Omega(u) = W(z(u), u)$ with respect to independent variables u is determined by the relation

$$d\Omega / du_i = W_{u_i}(z, u) + \sum_{q \in K_i} F_{u_i}(q, Z_q, U_q) p_q$$

Multipliers $p_i \in R^n$ are determined from the following system of linear algebraic equations (discrete conjugate problem):

$$p_i = W_{z_i}(z, u) + \sum_{q \in Q_i} F_{z_i}(q, Z_q, U_q) p_q$$

$$Q_i = \{j : 1 \le j \le n, \quad z_i \in Z_j\} \qquad K_i = \{j : 1 \le j \le n, \quad u_i \in U_j\}$$

Advantages of FAD-methodology

1). Canonical formulas

2). Precision

3). Effectiveness

The Cost functional approximation:

$$\Phi(K(T), C(T)) \cong F(k_0, k_1, \ldots, k_M, c_0, c_1, \ldots, c_M) =$$

$$= \sum_{j=1}^{J} \sum_{l=1}^{L-1} \sum_{i=1}^{I-1} \sum_{n=1}^{N-1} \left((T_{nil}^{j} - Y_{nil}^{j})^2 \cdot \mu_{nil}^{j} h_n^x h_i^y h_l^z \tau^j \right).$$

Direct Problem:

$x -$ direction:

$$T_{nil}^{j+1/3} = T_{nil}^{j} + a_n \frac{Q^x(T_{nil}^{j+1/3})}{C(T_{nil}^{j+1/3})} - b_n \frac{R^x(T_{nil}^{j+1/3})}{C(T_{nil}^{j+1/3})} \equiv \psi_{nil}^{j+1/3},$$

$y -$ direction:

$$T_{nil}^{j+2/3} = T_{nil}^{j+1/3} + \omega_i \frac{Q^y(T_{nil}^{j+2/3})}{C(T_{nil}^{j+2/3})} - d_i \frac{R^y(T_{nil}^{j+2/3})}{C(T_{nil}^{j+2/3})} \equiv \psi_{nil}^{j+2/3},$$

$z -$ direction:

$$T_{nil}^{j+1} = T_{nil}^{j+2/3} + e_l \frac{Q^z(T_{nil}^{j+1})}{C(T_{nil}^{j+1})} - f_l \frac{R^z(T_{nil}^{j+1})}{C(T_{nil}^{j+1})} \equiv \psi_{nil}^{j+1},$$

Conjugate Problem:

y − direction:

$$p_{nil}^{j+2/3} = \omega_i \cdot \frac{A^y\left(T_{nil}^{j+2/3}\right) \cdot C\left(T_{nil}^{j+2/3}\right) - Q^y\left(T_{nil}^{j+2/3}\right) \cdot C'_{T_{nil}^{j+2/3}}\left(T_{nil}^{j+2/3}\right)}{C^2\left(T_{nil}^{j+2/3}\right)} \cdot p_{nil}^{j+2/3} -$$

$$-d_i \cdot \frac{B^y(T_{nil}^{j+2/3}) \cdot C(T_{nil}^{j+2/3}) - R^y(T_{nil}^{j+2/3}) \cdot C'_{T_{nil}^{j+2/3}}(T_{nil}^{j+2/3})}{C^2(T_{nil}^{j+2/3})} \cdot p_{nil}^{j+2/3} +$$

$$+\omega_{i-1} \frac{B^y(T_{nil}^{j+2/3})}{C(T_{n,i-1,l}^{j+2/3})} \cdot p_{n,i-1,l}^{j+2/3} - d_{i+1} \cdot \frac{B^y(T_{nil}^{j+2/3})}{C(T_{n,i+1,l}^{j+2/3})} \cdot p_{n,i+1,l}^{j+2/3} + p_{nil}^{j+1}.$$

$x - \text{direction:}$

$$p_{nil}^{j+1/3} = a_n \cdot \frac{A^x\left(T_{nil}^{j+1/3}\right) \cdot C\left(T_{nil}^{j+1/3}\right) - Q^x\left(T_{nil}^{j+1/3}\right) \cdot C'_{T_{nil}^{j+1/3}}\left(T_{nil}^{j+1/3}\right)}{C^2\left(T_{nil}^{j+1/3}\right)} \cdot p_{nil}^{j+1/3} -$$

$$-b_n \cdot \frac{B^x\left(T_{nil}^{j+1/3}\right) \cdot C\left(T_{nil}^{j+1/3}\right) - R^x\left(T_{nil}^{j+1/3}\right) \cdot C'_{T_{nil}^{j+1/3}}\left(T_{nil}^{j+1/3}\right)}{C^2\left(T_{nil}^{j+1/3}\right)} \cdot p_{nil}^{j+1/3} +$$

$$+a_{n-1} \cdot \frac{B^x(T_{nil}^{j+1/3})}{C(T_{n-1,il}^{j+1/3})} \cdot p_{n-1,il}^{j+1/3} - b_{n+1} \cdot \frac{B^x(T_{nil}^{j+1/3})}{C(T_{n+1,il}^{j+1/3})} \cdot p_{n+1,il}^{j+1/3} + p_{nil}^{j+2/3}.$$

$z - \text{direction:}$

$$p_{nil}^{j} = e_l \cdot \frac{A^z(T_{nil}^{j}) \cdot C(T_{nil}^{j}) - Q^z(T_{nil}^{j}) \cdot C'_{T_{nil}^{j}}(T_{nil}^{j})}{C^2(T_{nil}^{j})} \cdot p_{nil}^{j} -$$

$$-f_l \cdot \frac{B^z\left(T_{nil}^{j}\right) \cdot C\left(T_{nil}^{j}\right) - R^z\left(T_{nil}^{j}\right) \cdot C'_{T_{nil}^{j}}\left(T_{nil}^{j}\right)}{C^2\left(T_{nil}^{j}\right)} \cdot p_{nil}^{j} +$$

$$+e_{l-1} \cdot \frac{B^z(T_{nil}^{j})}{C(T_{ni,l-1}^{j})} \cdot p_{ni,l-1}^{j} - f_{l+1} \frac{B^z(T_{nil}^{j})}{C(T_{ni,l+1}^{j})} \cdot p_{ni,l+1}^{j} + p_{nil}^{j+1/3} + \frac{\partial F}{\partial T_{nil}^{j}}.$$

Gradient of the Cost function

$$\frac{\partial F}{\partial k_m} = \sum_{g=0}^{J}\sum_{r=0}^{L}\sum_{q=0}^{I}\sum_{s=0}^{N}\left(W_{rqs}^{g}\frac{\partial K(T_{rqs}^{g})}{\partial k_m}\right) +$$

$$+\sum_{g=0}^{J-1}\sum_{r=0}^{L}\sum_{q=0}^{I}\sum_{s=0}^{N}\left(W_{rqs}^{g+1/3}\frac{\partial K(T_{rqs}^{g+1/3})}{\partial k_m} + W_{rqs}^{g+2/3}\frac{\partial K(T_{rqs}^{g+2/3})}{\partial k_m}\right),$$

$$\frac{\partial F}{\partial c_m} = \sum_{g=0}^{J}\sum_{r=0}^{L}\sum_{q=0}^{I}\sum_{s=0}^{N}\left(\Omega_{rqs}^{g}\frac{\partial C(T_{rqs}^{g})}{\partial c_m}\right) +$$

$$+\sum_{g=0}^{J-1}\sum_{r=0}^{L}\sum_{q=0}^{I}\sum_{s=0}^{N}\left(\Omega_{rqs}^{g+1/3}\frac{\partial C(T_{rqs}^{g+1/3})}{\partial c_m} + \Omega_{rqs}^{g+2/3}\frac{\partial C(T_{rqs}^{g+2/3})}{\partial c_m}\right),$$

Important facts:

1. The gradient is accurate for the selected approximation of the optimal control problem.
2. The conjugate variables used are the same for both components of gradient.

Results of Numerical Calculations

Several series of calculations were performed.

First series of calculations

The results were based on the fact that the function

$$\Lambda(x, y, z, t) = x + y + z + 3t + 0.5.$$

is the analytical solution to the equation

$$C(T(s,t))\frac{\partial T(s,t)}{\partial t} = div_s\left(K\left(T(s,t)\right) \cdot \nabla_s T(s,t)\right)$$

for $C(T) = 1,\qquad K(T) = T.$

Functions $w_0(s)$, $w_{\partial Q}(s,t)$ are the trace of $\Lambda(x, y, z, t)$ on the parabolic boundary of region $Q \times (0, \theta)$.

An "analytical" field $\Lambda(x, y, z, t)$ was used as an experimental temperature field $Y(x, y, z, t)$.

$$a = \min_{(s\in Q, t\in(0,\theta))} \Lambda(s,t)) = 0.5, \qquad b = \max_{(s\in Q, t\in(0,\theta))} \Lambda(s,t) = 6.5.$$

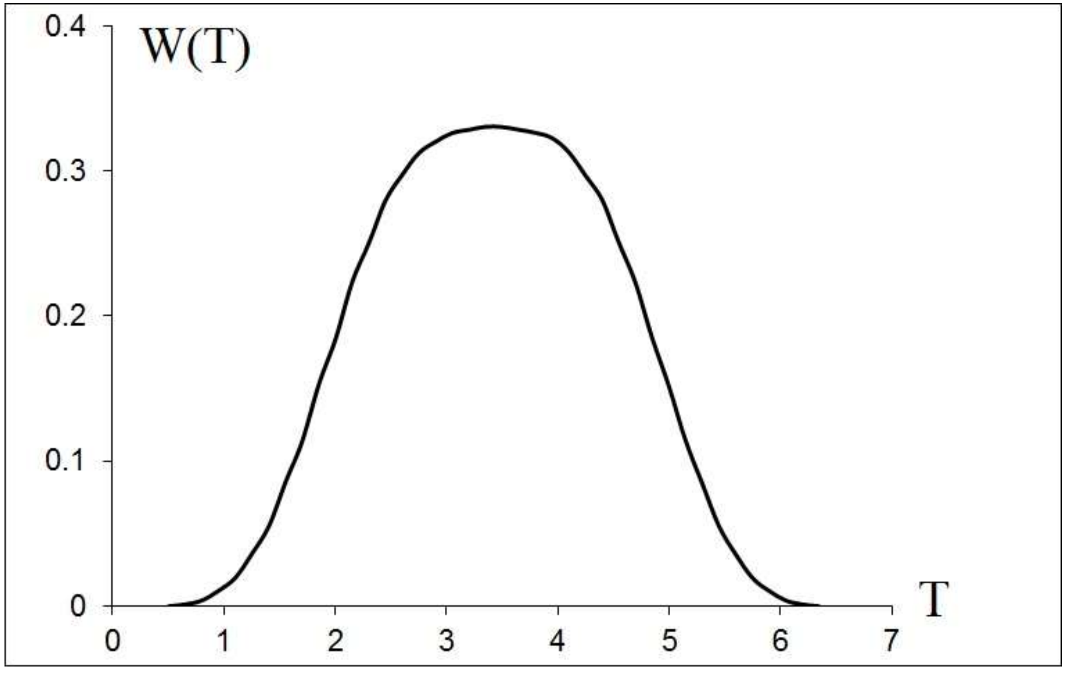

Fig. 1. Temperature distribution density.

Parameters:

1). $Q \times (0, \theta) = (0,1) \times (0,1) \times (0,1) \times (0,1)$.

2). The uniform grid with 30 intervals along the axes and 100 along the axis t was used.

3). The segment $[a, b]$ was partitioned into 40 intervals.

4). $\mu(x, t) = 1$.

First series, first example

$K(a) = a$ – *addition condition.*

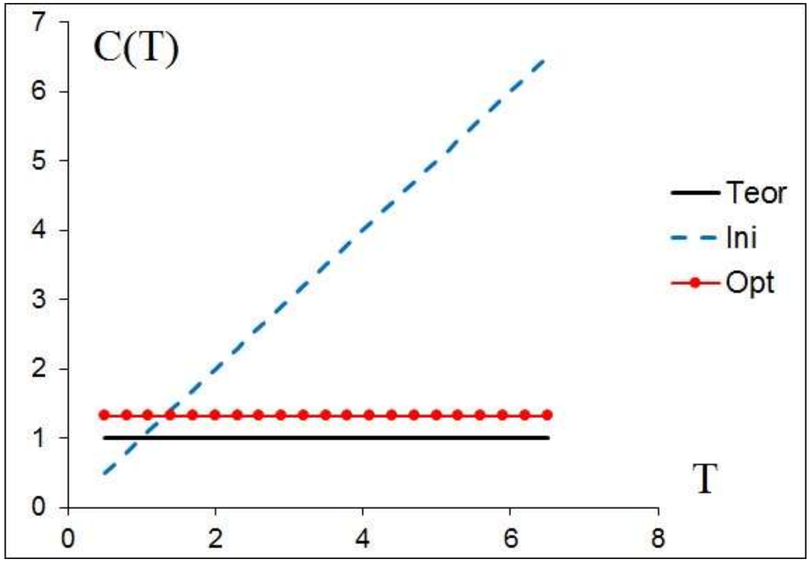

Fig. 2. Volumetric heat capacity.

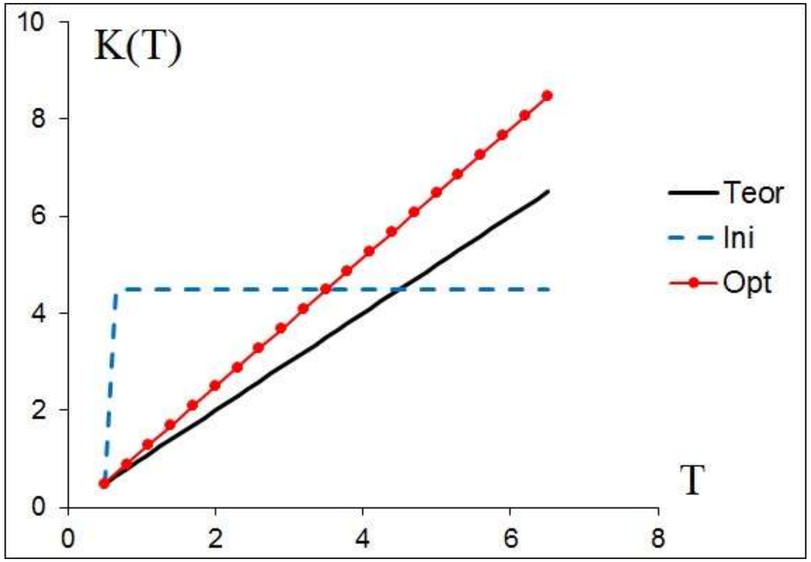

Fig. 3. Thermal conductivity.

1). The Cost function decreased from $3.39*10^{-03}$ at the initial approximation to $9.85*10^{-30}$.

2). The maximum relative deviation of the temperature field changed from $3.46*10^{-02}$ to $1.72*10^{-14}$.

3). The gradient modulus of the objective function decreased by 14 orders of magnitude.

Conclusion: *The solution is not unique*

First series, second example

$K(a) = a, \qquad C(a) = 1$ – *addition condition*.

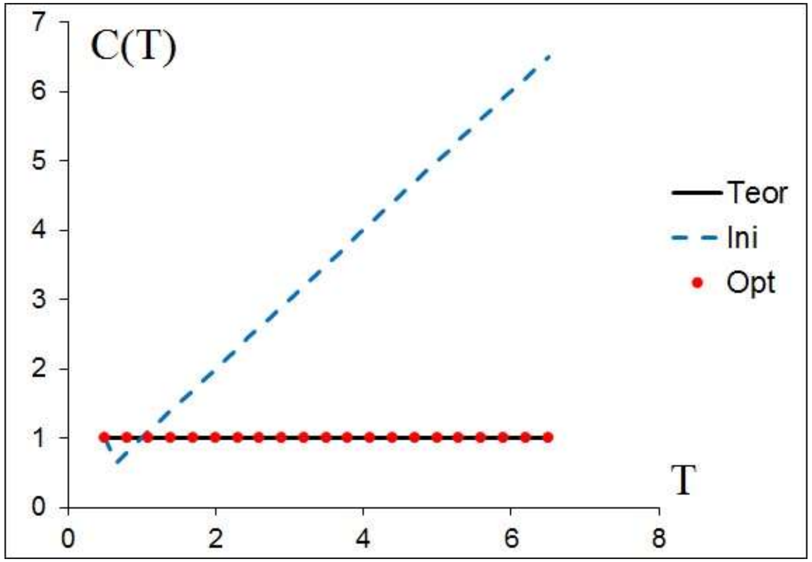

Fig. 4. Volumetric heat capacity.

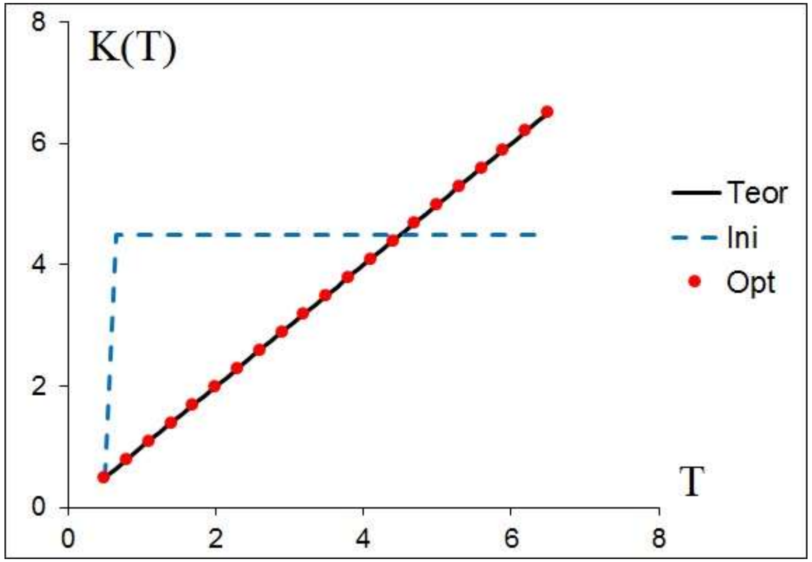

Fig. 5. Thermal conductivity.

1). The Cost function decreased from $3.39*10^{-03}$ at the initial approximation to $9.35*10^{-30}$.

2). The maximum relative deviation of the temperature field changed from $3.46*10^{-02}$ to $2.65*10^{-14}$.

3). The gradient modulus of the objective function decreased by 15 orders of magnitude.

Conclusion: *The solution is unique*

Second series of calculations

The experimental temperature field $Y(x, y, z, t)$ was constructed by solving the direct problem with special input data:

1). The temperature on the parabolic boundary of the region was equal to the trace of the function

$$\Lambda(x, y, z, t) = \sqrt{\frac{9 \cdot (x+1)^2 + 20y^2 + 25z^2}{9 - 8t}}$$

2). $C(T) = T$, $\quad K(T) = \begin{cases} 0.1 \cdot (T-3) \cdot (T-6) \cdot (T-7) + 3.4, & T \geq 3\,, \\ 1.2 \cdot (T-3) + 3.4\,, & T < 3\,. \end{cases}$

About field $Y(x, y, z, t)$:

$$a = \min_{(s\in Q, t\in(0,\theta))} \Lambda(s,t)) = 1, \qquad b = \max_{(s\in Q, t\in(0,\theta))} \Lambda(s,t) = 9.$$

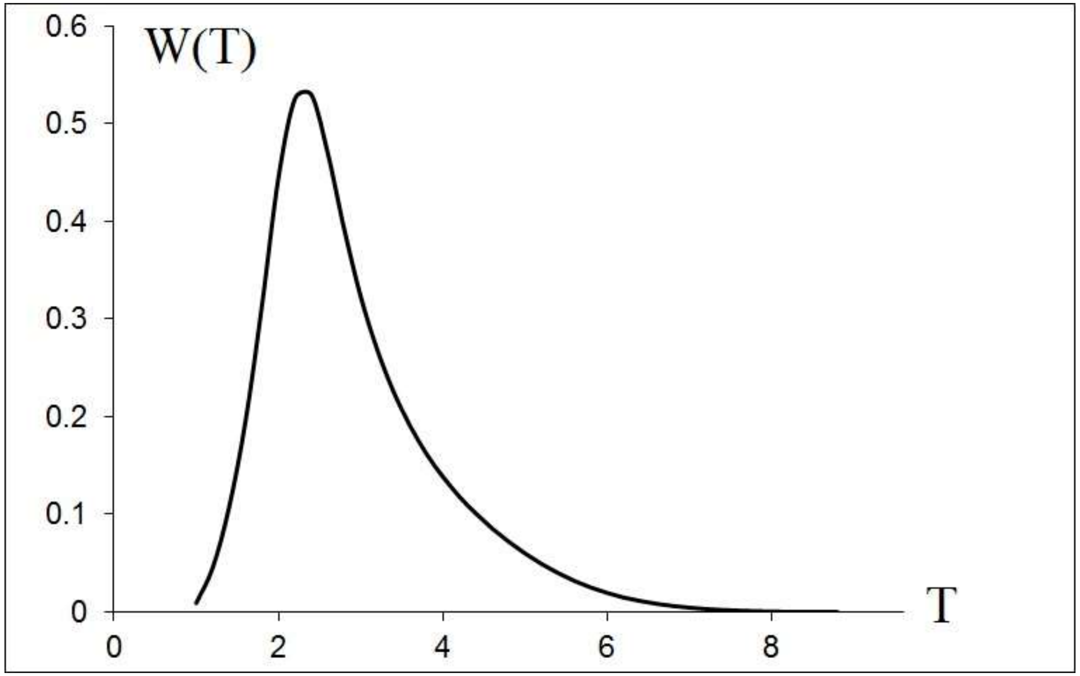

Fig. 6. Temperature distribution density.

There is too little experimental data outside the segment [1.5, 5.0].

There will be difficulties in restoring the desired parameters.

$K(5) = 3.8, \qquad C(5) = 5$ – *addition condition*.

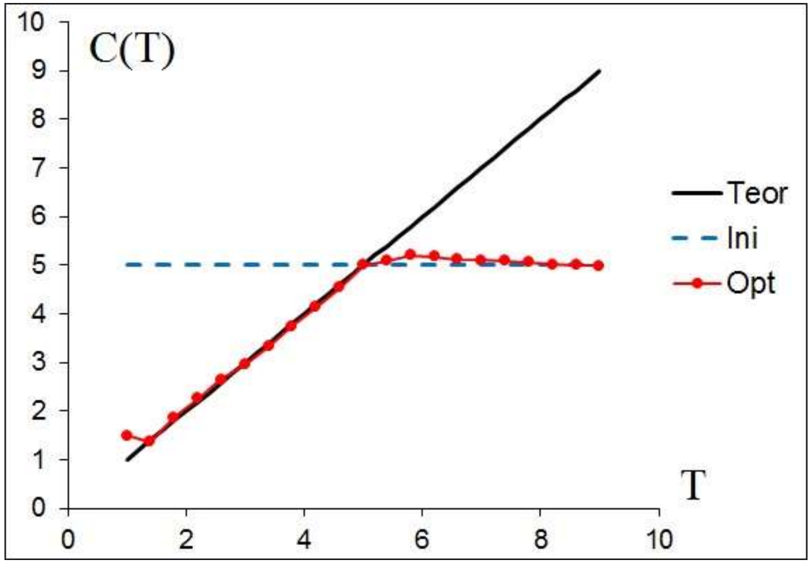

Fig. 7. Volumetric heat capacity.

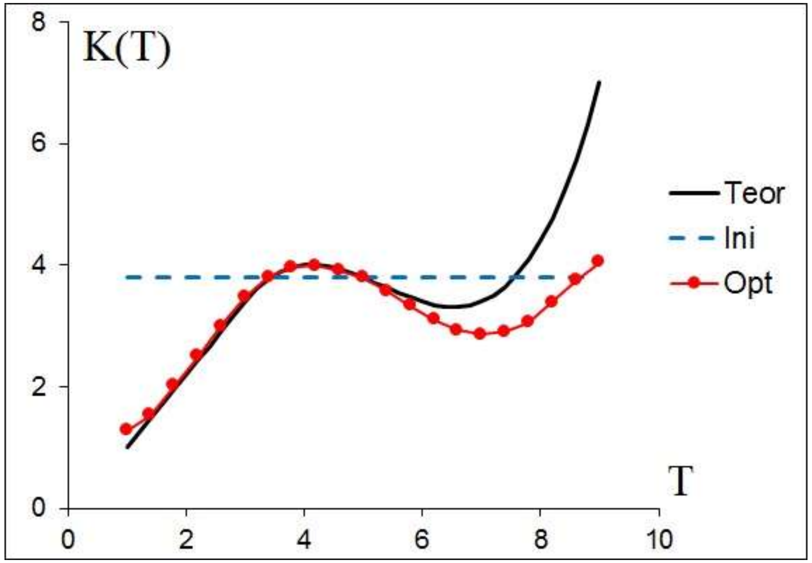

Fig. 8. Thermal conductivity.

1). The Cost function decreased from $2.21 \cdot 10^{-3}$ at the initial approximation to $1.87 \cdot 10^{-9}$.

2). The gradient modulus of the objective function decreased by 7 orders of magnitude.

Conclusions: *The parameters are not reconstructed where there is too little experimental data*

The solution is unique

Conclusions:

1). When considering the problem of simultaneous identification the volumetric heat capacity and the thermal conductivity over the temperature field in the three-dimensional case, the density of the distribution of experimental data along a given temperature segment plays an important role. For those temperature values at which there are few experimental data, the desired parameters are practically not identified.

2). The solution of the inverse problem may be not unique. To identify a single solution, it is recommended to impose additional conditions on the solution.

3). The use of the FAD technique allows one to obtain an exact gradient of the functional for the chosen approximation of the direct problem. This allows one to achieve the minimum of the functional (and construct control functions) with high accuracy using gradient optimization methods. Apparently, this approach is one of the ways to regularize the problem.

THANK YOU

FOR ATTANTION