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## IDENTIFIABILITY IN THE LARGE OF A LINEAR HEAT-CONDUCTION EQUATION

### SUBJECT TO CAUCHY BOUNDARY CONDITIONS

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The feasibility of simultaneously determining constant values of the specific heat, thermal conductivity, and heat-transfer coefficient from observations of a unique temperature field is studied.

An important problem in the theory of experimental design is the formulation of conditions such that the number of unknowns can be maximized for a given volume of measurements. In the practice of thermophysical investigations [1, 2] the comprehensive determination of the properties of a body is usually limited to two coefficients: the specific heat and the thermal conductivity. Extending the statement of the problem, we now explore the feasibility of simultaneously determining the values of the specific heat, thermal conductivity, and heat-transfer coefficient from observations of a unique temperature field.

To solve this problem we use an approach proposed earlier [3]. It is based on an investigation of the one-to-one correspondence between the unknown parameters and the state function of the model in question. Then the determination of the class of temperature fields for which the one-to-one correspondence fails could provide the basis for simultaneously identifying several parameters of the thermal model according to the conditions for the elimination of observations of an unidentifiable state. From the point of view of uniqueness of the solution of inverse coefficient problems and within the framework of linear models the present study continues work begun earlier [4], where it was proposed that the conditions for preservation of the one-to-one correspondence be specified as identifiability in the large and the family of coefficients corresponding to one particular solution of the boundary-value problem was expressed as an ambiguity subset.

We now consider a linear heat-conduction equation whose associated boundary conditions contain unknown coefficients. Let it be supposed that the following boundary-value problem is given in the domain of variation of the independent variables  $Q_T = \{(x, t) : 0 < x < 1, 0 < t < T\}$ :

$$\begin{aligned}
 a_1 \frac{\partial u}{\partial t} &= a_2 \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad (x, t) \in Q_T, \\
 u|_{t=0} &= \varphi(x), \quad 0 < x < 1, \\
 a_3(u|_{x=0} - v_0) - a_2 \frac{\partial u}{\partial x} \Big|_{x=0} &= 0, \quad 0 < t < T, \\
 a_3(u|_{x=1} - v_1) + a_2 \frac{\partial u}{\partial x} \Big|_{x=1} &= 0, \quad 0 < t < T,
 \end{aligned} \tag{1}$$

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where  $f(x, t) \in C^{2,1}(\bar{Q}_T)$ ,  $\varphi(x) \in C^2[0, 1]$ ,  $v_{0,1}(t) \in C^1[0, T]$  are known differentiable functions, and  $\alpha_{1,2,3} = \text{const} > 0$  are the thermophysical coefficients: specific heat, thermal conductivity, and heat-transfer coefficient.

It is assumed that the initial data of the model (1) satisfy the requirements of the existence of a unique differentiable solution. In this case the failure of one-to-one correspondence between the coefficients  $\alpha_{1,2,3}$  and the temperature field  $u(x, t)$  is expressed in the following theorem.

**THEOREM 1.** A solution of problem (1), unidentifiable in the large, has the form

$$u^* = \rho^{-1} \int_0^t f^*(x, \tau) d\tau + \varphi(x), \quad (x, t) \in Q_T, \quad (2)$$

for the existence of which the necessary and sufficient conditions are: specification of a family

$$\lambda_1 a_1 - a_2 = \lambda_1 \rho, \quad \lambda_2 a_3 - a_2 = 0, \quad (3)$$

consistency of the boundary conditions

$$\varphi|_{x=0} - \lambda_2 \frac{d\varphi}{dx} \Big|_{x=0} = v_0|_{t=0}, \quad \varphi|_{x=1} + \lambda_2 \frac{d\varphi}{dx} \Big|_{x=1} = v_1|_{t=0}, \quad (4)$$

and satisfaction of the following conditions by the function  $f^*$ :

$$\frac{\partial f^*}{\partial t} = \lambda_1 \frac{\partial^2 f^*}{\partial x^2}, \quad (x, t) \in Q_T, \quad (5)$$

$$f^*|_{t=0} = \lambda_1 \rho \frac{d^2 \varphi}{dx^2}, \quad 0 < x < 1, \quad (6)$$

$$f^*|_{x=0} - \lambda_2 \frac{\partial f^*}{\partial x} \Big|_{x=0} = \rho \frac{dv_0}{dt}, \quad 0 < t < T, \quad (7)$$

$$f^*|_{x=1} + \lambda_2 \frac{\partial f^*}{\partial x} \Big|_{x=1} = \rho \frac{dv_1}{dt}, \quad 0 < t < T, \quad (8)$$

where  $\lambda_{1,2}, \rho = \text{const}$ .

**Proof of the Theorem. Necessity.** Let us assume that two vectors  $a' \neq a''$ , where  $a'' = \{a_1, a_2, a_3\}$ , correspond to a single solution  $u^*(x, t) \in C^{2,1}(\bar{Q}_T)$ . Then we can deduce

$$(a_1 - a_1') \frac{\partial u^*}{\partial t} = (a_2' - a_2'') \frac{\partial^2 u^*}{\partial x^2}, \quad (x, t) \in Q_T,$$

$$(a_3' - a_3'') (u^*|_{x=0} - v_0) = (a_2' - a_2'') \frac{\partial u^*}{\partial x} \Big|_{x=0}, \quad 0 < t < T,$$

$$(a_3' - a_3'') (u^*|_{x=1} - v_1) = - (a_2' - a_2'') \frac{\partial u^*}{\partial x} \Big|_{x=1}, \quad 0 < t < T.$$

From this result we infer linear dependence of the differential terms of the given problem

$$\frac{\partial u^*}{\partial t} = \lambda_1 \frac{\partial^2 u^*}{\partial x^2}, \quad (x, t) \in Q_T \quad (9)$$

and the terms of the boundary conditions

$$u^*|_{x=0} - v_0 = \lambda_2 \frac{\partial u^*}{\partial x} \Big|_{x=0}, \quad 0 < t < T; \quad (10)$$

$$u^*|_{x=1} - v_1 = -\lambda_2 \frac{\partial u^*}{\partial x} \Big|_{x=1}, \quad 0 < t < T.$$

We use (9) to transform the initial heat-conduction equation to the form

$$\frac{\partial u^*}{\partial t} = \rho^{-1} f, \quad (x, t) \in Q_T, \quad (11)$$

where the expression

$$\rho = a_1 - \frac{a_2}{\lambda_1} \quad (12)$$

determines the nature of the relationship between the specific heat and thermal conductivity coefficients of problem (1) generating the unidentifiable temperature field (2).

Substituting the solution (2) into condition (9), we obtain

$$f = \lambda_1 \int_0^t \frac{\partial^2 f}{\partial x^2} d\tau + \lambda_1 \rho \frac{d^2 \varphi}{dx^2}, \quad (x, t) \in Q_T, \quad (13)$$

whence we arrive at (5) and (6). Applying the boundary operators in succession to the function (2), we find

$$a_3 \left( f|_{x=0} - \rho \frac{dv_0}{dt} \right) - a_2 \frac{\partial f}{\partial x} \Big|_{x=0} = 0, \quad 0 < t < T,$$

$$a_3 \left( f|_{x=1} - \rho \frac{dv_1}{dt} \right) + a_2 \frac{\partial f}{\partial x} \Big|_{x=1} = 0, \quad 0 < t < T,$$

$$a_3 (\varphi|_{x=0} - v_0|_{t=0}) - a_2 \frac{d\varphi}{dx} \Big|_{x=0} = 0,$$

$$a_3 (\varphi|_{x=1} - v_1|_{t=0}) + a_2 \frac{d\varphi}{dx} \Big|_{x=1} = 0.$$

These expressions are transformed to (7), (8), and (4), and the coefficients of the boundary conditions turn out to be related by the equation

$$\lambda_2 a_3 - a_2 = 0. \quad (14)$$

Thus, from the hypothesis of the existence of different coefficients corresponding to the same solution we deduce the satisfaction of conditions (3)-(8).

Sufficiency. In the domain  $Q_T$  let us consider the function

$$w(x, t) = \frac{\partial u}{\partial t} - \lambda_1 \frac{\partial^2 u}{\partial x^2} \in C^{2,1}(\bar{Q}_T),$$

whose existence and differential properties follow from the differentiability of the solution  $u(x, t) \in C^{2,1}(\bar{Q}_T)$  and  $f(x, t) \in C^{2,1}(\bar{Q}_T)$ . Now, applying the operators  $\partial/\partial t$  and  $\partial^2/\partial x^2$  to the heat-conduction equation and then comparing the results according to (5), we obtain the homogeneous equation

$$a_1 \frac{\partial w}{\partial t} = a_2 \frac{\partial^2 w}{\partial x^2}, \quad (x, t) \in Q_T.$$

If we choose from the set of coefficients of problem (1) those which are interrelated by condition (12), then the function  $w(x, t)$  is expressed in the same way as  $w = \left( f - \lambda_1 \rho \frac{\partial^2 u}{\partial x^2} \right) / a_1$

or  $w = \left( \lambda_1 f - \lambda_1 \rho \frac{\partial u}{\partial t} \right) / a_2$ . From these two expressions, given the satisfaction of (6)-(8) and (14), we obtain

$$w|_{t=0} = 0, \quad 0 < x < 1,$$

$$w|_{x=0} - \lambda_2 \frac{\partial w}{\partial x} \Big|_{x=0} = 0, \quad 0 < t < T,$$

$$w|_{x=1} + \lambda_2 \frac{\partial w}{\partial x} \Big|_{x=1} = 0, \quad 0 < t < T.$$

Hence it follows that the function  $w(x, t)$  is identically zero and so condition (9) holds. The linear dependence of (10) is inferred directly from the boundary conditions with regard for (14).

To demonstrate the sufficiency of conditions (9) and (10) for violating the one-to-one correspondence we analyze the functional

$$J(\alpha) = \int_{Q_T} \left( a_1 \frac{\partial u}{\partial t} - a_2 \frac{\partial^2 u}{\partial x^2} - f \right)^2 dxdt + \int_0^T \left\{ \left[ a_3 (u|_{x=0} - v_0) - a_2 \frac{\partial u}{\partial x} \Big|_{x=0} \right]^2 + \left[ a_3 (u|_{x=1} - v_1) + a_2 \frac{\partial u}{\partial x} \Big|_{x=1} \right]^2 \right\} dt.$$

From the condition for its minimum we determine the vector  $\alpha$  for which the specified function  $u(x, t)$  is a solution of problem (1). In this case the satisfaction of (9) and (10) implies a linear dependence of the equations of the system expressing the minimum of the functional  $J(\alpha)$ . Consequently, a nonunique vector  $\alpha$  exists, corresponding to one solution of the stated problem. This completes the proof.

We now analyze the foregoing results. Conditions (3)-(8) indicate when, and only when, a one-to-one correspondence does not exist between the coefficients of the investigated model and its state function. Here the requirement of satisfaction of (4)-(8) is necessary in order for the family (3) to describe the ambiguity subset of problem (1) and for its solution to belong to the subspace of unidentifiable functions. Then the failure of at least one of these conditions will imply uniqueness of the relation between the coefficients  $\alpha_{1,2,3} = \text{const}$  and the temperature field  $u(x, t) \in C^{2,1}(\bar{Q}_T)$ . From this result we infer the possibility of simultaneous identification of constant values of the specific heat, thermal conductivity, and heat-transfer coefficient if the observations are not made on temperatures of the form (2). Otherwise a solution of the inverse problem for the model (1) is obtainable only correct to within the family (3).

From the point of view of invariant properties, the existence of the family (3) implies that the temperature field can remain unchanged if (4)-(8) are satisfied and if the thermo-physical properties of the bar and the heat transfer at its boundaries are transformed according to (3). For example, the solution of problem (1) with the initial data  $a_1 = 3$ ,  $a_2 = 1$ ,  $a_3 = \alpha$ ,  $f = 1$ ,  $\varphi = x(x-1)$ ,  $v_{0,1} = t + \alpha^{-1}$  is preserved for any variations of  $\alpha > 0$ .

It follows from the form of the family (3) that the solution (2) is invariant under the transformation  $a_1'' = a_1' + c$ ,  $a_2'' = a_2' + c\lambda_1$ ,  $a_3'' = a_3' + \frac{c\lambda_1}{\lambda_2}$ ,  $c = \text{const}$ , which represents the translation group acting on the set of coefficients of the boundary-value problem (1).

In contrast with the problem statement discussed previously [4] with a domain of definition that does not depend on the unknown coefficients, the parameters of the family (3) are not always unique. The value of  $\lambda_2$  is arbitrary if the function  $f^*$  satisfies Eq. (5) subject to the conditions

$$\frac{\partial f^*}{\partial x} \Big|_{x=0} = \frac{\partial f^*}{\partial x} \Big|_{x=1} = 0, \quad 0 < t < T; \quad \int_0^1 f^*|_{t=0} dx = 0,$$

with which are associated the boundary functions

$$v_0 = \rho^{-1} \int_0^t f^*|_{x=0} d\tau + v, \quad 0 < t < T; \quad v_1 = \rho^{-1} \int_0^t f^*|_{x=1} d\tau + \lambda_1^{-1} \rho^{-1} \int_0^1 \int_0^z f^*|_{t=0} dz d\xi + v, \quad 0 < t < T$$

and the initial temperature distribution

$$\varphi = \lambda_1^{-1} \rho^{-1} \int_0^x \int_0^z f^*|_{t=0} dz d\xi + c, \quad 0 < x < 1,$$

where  $c$  and  $v$  are arbitrary constants. Then at any time the solution of problem (1) will have the form

$$\frac{\partial u^*}{\partial x} \Big|_{x=0} = \frac{\partial u^*}{\partial x} \Big|_{x=1} = 0, \quad 0 < t < T.$$

In such cases it is impossible to indicate the heat-transfer coefficients  $\alpha_3$  unambiguously. Consequently, the ambiguity subset of problem (1) can contain a nonunique family.

The following consequence of the form of the family (3) is important in practice.

**COROLLARY 1.** If the heat-transfer coefficients  $\alpha_3$  is given, the model (1) is identifiable in the large for any values of  $f$ ,  $\varphi$ , and  $v_{0,1}$  that ensure the existence of a unique temperature field.

In the given situation we have expressed the possibility of uniquely determining the specific heat and thermal conductivity when the inverse problem is generated by Newton's formulation with a known heat transfer at the boundary.

Also important for the solution of applied problems is the following.

**COROLLARY 2.** The ambiguity subset of problem (1) for arbitrary values of the function  $f \neq 0$  is empty if constant boundary functions  $v_{0,1}$  and a linear initial distribution  $\varphi$  are given.

The corollary, like the preceding results, can be used as a basis for selecting experimental arrangements aimed at the simultaneous determination of several thermophysical parameters. For example, the temperature field needed for identifying simultaneously by means of the model (1) the specific heat, thermal conductivity, and heat-transfer coefficient of a bar with a uniform initial state and a constant ambient temperature can be created by any internal heat source, including Joule heat with a constant power.

Of unquestionable interest for the theory of inverse problems is the solution of the problem of whether it is possible to determine both the thermophysical properties of a bar and the heat fluxes at its boundaries. Theorem 1 shows that if the temperature field is identifiable in the large, then the model (1) admits simultaneous identification of the thermophysical properties and boundary heat fluxes. We thus arrive at the following.

**COROLLARY 3.** For the simultaneous determination of the specific heat, thermal conductivity, and boundary heat fluxes of the model (1) it is necessary that the observed temperature field be identifiable in the large.

In the special case when an experiment is based on the model of transient symmetrical heating of a bar with a thermally insulated side surface

$$\begin{aligned} a_1 \frac{\partial u}{\partial t} &= a_2 \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad (x, t) \in Q_T, \\ u|_{t=0} &= \varphi(x), \quad 0 < x < 1, \\ \frac{\partial u}{\partial x} \Big|_{x=0} &= 0, \quad -a_2 \frac{\partial u}{\partial x} \Big|_{x=1} = q(t), \quad 0 < t < T, \end{aligned}$$

the set of parameters  $\{a_{1,2}, q\}$  can be determined if the observed temperature field does not belong to the subspace of unidentifiable solutions described by the quadrature (2). This result attests to the possibility of simplifying considerably the technological configuration of the experiment by including difficult-to-measure quantities such as, for example, the heat fluxes admitted to the object and its thermophysical properties among the unknown parameters.

Having investigated a model with homogenous boundary conditions, we now turn to a formulation with inhomogeneities at the boundaries. Let it be supposed that the following model is given in the domain  $Q_T = \{(x, t) : 0 < x < 1, 0 < t < T\}$ :

$$\begin{aligned} a_1 \frac{\partial u}{\partial t} &= a_2 \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad (x, t) \in Q_T, \\ u|_{t=0} &= \varphi(x), \quad 0 < x < 1, \\ a_3 u|_{x=0} - a_2 \frac{\partial u}{\partial x} \Big|_{x=0} &= q_0(t), \quad 0 < t < T, \\ a_3 u|_{x=1} + a_2 \frac{\partial u}{\partial x} \Big|_{x=1} &= q_1(t), \quad 0 < t < T, \end{aligned} \tag{15}$$

where  $f(x, t) \in C^{2,1}(\bar{Q}_T)$ ,  $\varphi(x) \in C^2[0, 1]$ ,  $q_{0,1}(t) \in C[0, T]$  are known functions. In this case the following is pertinent to the given problem.

**THEOREM 2.** A solution of problem (15), unidentifiable in the large, has the form

$$u^* = \rho_1^{-1} \int_0^t f^*(x, \tau) d\tau + \varphi(x), \quad (x, t) \in Q_T, \tag{16}$$

for the existence of which the necessary and sufficient conditions are: specification of a family

$$\lambda_1 a_1 - a_2 = \lambda_1 \rho_1, \quad \lambda_2 a_3 - a_2 = \rho_2,$$

and satisfaction of the conditions

$$\begin{aligned} \frac{\partial f^*}{\partial t} &= \lambda_1 \frac{\partial^2 f^*}{\partial x^2}, \quad (x, t) \in Q_T, \\ f^*|_{t=0} &= \lambda_1 \rho_1 \frac{d^2 \varphi}{dx^2}, \quad 0 < x < 1, \\ f^*|_{x=0} - \lambda_2 \frac{\partial f^*}{\partial x} \Big|_{x=0} &= 0, \quad 0 < t < T, \\ f^*|_{x=1} + \lambda_2 \frac{\partial f^*}{\partial x} \Big|_{x=1} &= 0, \quad 0 < t < T, \\ q_0 &= \frac{\rho_2}{\rho_1} \int_0^t \frac{\partial f^*}{\partial x} \Big|_{x=0} d\tau + \rho_2 \frac{d\varphi}{dx} \Big|_{x=0}, \quad 0 < t < T, \\ q_1 &= -\frac{\rho_2}{\rho_1} \int_0^t \frac{\partial f^*}{\partial x} \Big|_{x=1} d\tau - \rho_2 \frac{d\varphi}{dx} \Big|_{x=1}, \quad 0 < t < T, \\ \varphi|_{x=0} - \lambda_2 \frac{d\varphi}{dx} \Big|_{x=0} &= 0, \quad \varphi|_{x=1} + \lambda_2 \frac{d\varphi}{dx} \Big|_{x=1} = 0, \end{aligned}$$

where  $\lambda_{1,2}, \rho_{1,2} = \text{const.}$

The theorem can be proved by a scheme similar to the one used in the case discussed above.

The results obtained in Theorem 2 indicate that inhomogeneities in the boundary conditions as well as in the heat-conduction equation do not exclude instances of the failure of one-to-one correspondence. Consequently, the requirement of inhomogeneity of the mathematical model is not a sufficient condition for identifiability. The final answer can only be given by the properties of the observed temperature field, which, in order for the solution of the inverse problem to be unique, must not be described by the quadrature (16).

The formulation of a problem of the form (15) makes it possible to investigate an important practical experimental arrangement for the determination of thermophysical properties, which is expressed by the heat-conduction equation and Cauchy-type boundary conditions:

$$\begin{aligned} a_1 \frac{\partial u}{\partial t} &= a_2 \frac{\partial^2 u}{\partial x^2}, \quad (x, t) \in Q_T, \\ u|_{t=0} &= \varphi(x), \quad 0 < x < 1, \\ -a_2 \frac{\partial u}{\partial x} \Big|_{x=0} &= q_0(t), \quad -a_2 \frac{\partial u}{\partial x} \Big|_{x=1} = q_1(t), \quad 0 < t < T. \end{aligned}$$

In this case homogeneity of the boundary conditions, i.e.,  $q_{0,1} \equiv 0$ , is necessary and sufficient for the existence of a solution  $u^*$  unidentifiable in the large. Accordingly, we have the following.

**COROLLARY 4.** A homogeneous linear heat-conduction equation is identifiable in the large if at least one inhomogeneous Cauchy boundary condition is given.

This result shows that the familiar method of a surface source [1, 2] can be used to determine both the specific heat and thermal conductivity from observations of a unique field. It is possible in this connection to reduce considerably the volume of experimental investigations and measurements by solving the appropriate inverse problem. It must be noted that the subject here is the conceptual possibility of simultaneous identification, because the preservation of one-to-one correspondence does not preclude other cases of ambiguity of the solution of inverse problem such as, for example, those associated with the discreteness of the observations.

Summarizing the results, we draw the following conclusions. In the experimental investigation of heat-transfer processes on the basis of a limited volume of initial data it is possible to determine simultaneously a set of parameters that do not violate the one-to-one correspondence with given observations. The experimental assurance of the conditions necessary for this objective permits the specific heat and thermal conductivity to be determined simultaneously without using volume heat sources, or likewise the thermophysical properties and transient boundary heat fluxes, and additionally the heat-transfer coefficient to be reconstructed. What this means in practice is the possibility of enlarging the volume of information obtainable in the interpretation of experimental results by conventional methods. It must also be borne in mind that among the solutions of the heat-conduction equation there exists a subset that imparts ambiguity to the determination of the coefficients of the mathematical model. The existence of that subset is attributable to the invariant properties of the solution of the boundary-value problem with respect to its coefficients. The resulting necessary conditions for the existence of an unidentifiable temperature field can be applied directly in practice.

#### NOTATION

$x$ , space coordinate;  $t$ , time;  $Q_T$ , domain of independent variables;  $T$ , upper time limit;  $\alpha_1$ , specific heat;  $\alpha_2$ , thermal conductivity;  $\alpha_3$ , heat-transfer coefficient;  $f$ , power of volume heat sources;  $\varphi$ , initial temperature distribution;  $v_{0,1}$ , boundary functions;  $q, q_0, q_1$ , heat flux;  $u$ , temperature field;  $u^*$ , unidentifiable state;  $\lambda_{1,2}, \rho, \rho_1, \rho_2$ , parameters of family from ambiguity subset;  $C^1, C^2, C^{2,1}$ , classes of differentiable functions.

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#### MATHEMATICAL SIMULATION OF THERMOGRAVITATIONAL CONVECTION IN SOLIDIFICATION OF LIQUID STEEL

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The thermal and hydrodynamic phenomena accompanying crystallization of liquid steel are analyzed numerically.

It is well known that the major portion of defects in castings develop during the phase transition of the alloy from the liquid to the solid state. Direct experimental study of the thermal and especially the hydrodynamic phenomena accompanying the steel crystallization process is difficult because of the thermal and chemical aggressiveness of liquid steel. Thus, the role of mathematical simulation becomes important in study of this process.

Metallic alloys are inclined to produce dendrite forms of crystal growth, leading to formation of a two-phase zone which is a mixture of liquid alloy and branches of the growing dendrites. Thus, within the solidifying alloy one can always distinguish three regions with different aggregate metal states — a zone of completely solidified metal, a zone of liquid alloy, and a two-phase zone separating the former ones (Fig. 1).

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