Modifications of method for solving inverse heat and mass transfer problems

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Abstract

The paper proposes a modification of the multigrid method for solving the main classes of inverse heat and mass transfer problems, which belong to the class of ill-posed problems of mathematical physics, which in turn are of great importance for applied heat engineering research. The modification of the multigrid method is applied to direct heat and mass transfer problems, due to the fact that solving one inverse problem requires repeated solving of the direct problem, regardless of which optimizer is used to find the global extremum of the quadratic functional, which underlies the inverse heat and mass transfer problems. This approach allows formalizing the problem of parameter identification and ensuring the possibility of its solution by optimization methods of global multidimensional optimization. This paper also proposes numerical schemes based on difference approximations, which guarantee the stability of the computational process and the convergence of the obtained results. The effectiveness of the developed approach was tested on model examples, which showed its ability to significantly reduce the number of calculations to find a solution to a specific problem, while leaving the same error that arises during approximate calculations. The results obtained demonstrate the possibility of using the proposed approach for modeling and optimizing heat engineering processes in industrial and muffle furnaces, the mathematical model for which is used in work where high-precision control of temperature distribution is required. The practical significance of the study is to create a basis for the development of new systems for monitoring and controlling thermal regimes. This will ensure increased efficiency and reliability of energy technology processes. Also, the practical significance of the obtained results lies in the application of the developed methods, models and tools in the tasks of monitoring and diagnosing complex processes, including in the modeling and localization of environmental pollutants.

Keywords

inverse heat and mass transfer problems, partial differential equations, Newton's method, swarm intelligence, finite difference method, multigrid method

1. Introduction

In the conditions of rapid development of modern information technologies and computing facilities, the demand for the development of new and modification of existing methods and algorithms for solving inverse problems in the optimization mathematical formulation has grown rapidly [1]. Such problems make it possible to automate the process of designing complex objects, their systems and components of these systems in order to obtain reliable systems in various difficult conditions of use. It should be noted that such problems make it possible to perform an analysis of existing physical objects in order to determine their residual service life.

Inverse problems are an important class of problems in applied mathematics and mathematical physics, because they allow, based on known observations, experimental data or monitoring results, to restore unknown characteristics of the studied object, process or environment [1, 2]. Unlike direct problems, in which the consequences are determined based on given parameters,

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inverse problems are aimed at finding unknown input data from known output observations. This approach is of fundamental importance in science and technology, as it allows for the analysis and reproduction of those characteristics of objects that cannot be directly measured or observed. In modern conditions, inverse problems are widely used in many industries: from technical diagnostics and non-destructive testing to medicine, environmental monitoring, and energy [2–4]. For example, using inverse problems, it is possible to restore the temperature distribution or heat flows in solids, determine the physical and mechanical properties of materials, detect defects in structures, track the state of energy infrastructure objects, or determine environmental parameters based on sensor system data [1, 5]. On the other hand, solving inverse problems is traditionally associated with a number of difficulties. Such problems belong to the class of incorrectly posed problems in the Hadamard sense, since even minor errors in the initial or experimental data can lead to significant distortions in the results [1]. This necessitates the development of special methods of regularization, stabilization and optimization, which would ensure the correctness of solutions and the stability of algorithms to errors and noise in the data. Therefore, mathematical models and algorithmic approaches for solving inverse problems require constant improvement, taking into account the latest achievements in the field of computational mathematics, optimization and intelligent information technologies [6].

This paper considers a special example of the application of methods for solving inverse problems, which consists in the analysis and optimization of operating modes of muffle and industrial furnaces, examples of which are given in Figure 1. Muffle and industrial furnaces are widely used in metallurgy, mechanical engineering, ceramic production and other industries where prolonged heating of materials to high temperatures under controlled conditions is required [5–7]. For such units, an important task is to maintain a uniform temperature distribution in the working volume of the furnace, which ensures the uniformity of the physical and mechanical properties of the finished product. The formulation of the problem in the inverse formulation allows us to determine the optimal heat transfer parameters, design characteristics of the muffle or thermal insulation, as well as energy supply modes to achieve the specified technological indicators.

Figure 1: Examples of industrial and muffle furnaces that are actively used in production

Industrial furnaces are characterized by high energy consumption and complex dynamics of thermal processes, so their modeling requires taking into account nonlinear equations of heat and mass transfer, convection and radiation [8, 9]. The use of inverse problems in combination with optimization methods allows you to identify thermal parameters, diagnose defects and increase the energy efficiency of equipment. In particular, thanks to modern optimization algorithms, it is possible not only to predict the condition of furnaces and the residual resource of their components, but also to provide adaptive control of heating processes in order to reduce energy consumption and improve the quality of the final product.

Modern engineering systems and technological processes are characterized by multiparametricity, nonlinearity and complex dynamics. Performing the analysis of such systems in direct formulation is resource-intensive and often impractical. Instead, formulating the problem in the form of an inverse problem allows you to determine the optimal parameters or structure of the object, focusing directly on the desired output characteristics. This opens up wide opportunities for building reliable and durable systems capable of operating in difficult operating conditions.

An equally important aspect is the use of inverse problem solving methods for analyzing the residual resource of physical objects and structures [8–10]. In modern conditions, when a significant part of the infrastructure and industrial equipment is in operation for a long time, the task of predicting the residual resource acquires strategic importance. The use of identification methods and mathematical modeling based on experimental data allows not only to assess the current state of the object, but also to predict possible failures, prevent emergency situations and increase operational safety [1, 11, 12].

An important direction of modern research is the combination of classical optimization methods with the latest approaches of artificial intelligence and swarm algorithms (Figure 2) [10].

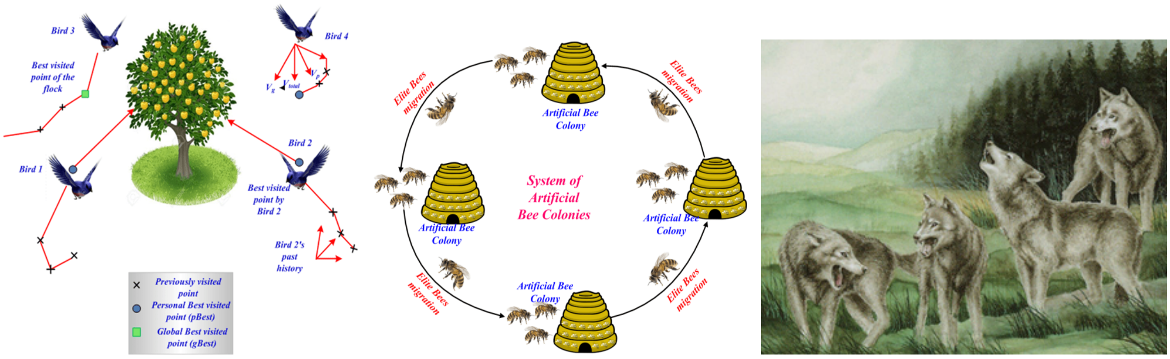

Figure 2: Examples of well-known current methods of global optimization in complex systems that have natural principles of operation

It should be noted that in today's conditions, the use of genetic algorithms, particle swarm methods, ant colonies, differential evolution and other metaheuristic algorithms for global optimization makes it possible to significantly expand the fields of science and technology, in particular, in complex design problems, combinatorial optimization problems, etc. [10]. Such methods are flexible, avoid getting stuck in local minima, and also provide high-quality optimization results even in cases where analytical or classical numerical approaches become ineffective.

2. Technical problem statement

The technical task is to build a mathematical model for optimizing the operation of an industrial / muffle furnace, which contains an object in the area G, which is located in a fixed position of the furnace itself. In order to increase its efficiency, this furnace contains heat sources, which are specified in the form of point heaters on an electric basis. Electric furnace heaters are also located in the furnace in predetermined geometric coordinates. It is necessary to determine what temperatures need to be applied to these point heaters so that the temperature on the object furnace is as close as possible to the predetermined T_{actual}. The constructed mathematical model must be implemented programmatically, choosing an optimization method. Since the constructed mathematical model refers to inverse models, since the cause-and-effect relationships of the temperature distribution in the industrial furnace are lost, it is reduced to the repeated use of the procedure for solving direct problems, which are described in the form of second-order partial differential equations. It is necessary to construct an additional method for solving the direct problem based on the multi-grid difference method in order to reduce the number of calculations required to obtain a solution to the problem of determining the optimal temperatures of the furnace heaters. For simplicity, the number of furnace heaters can be taken as fixed. In the following description, their number will be equal to six.

3. Mathematical formulation of the problem

The optimization problem is to find a global functional that has the classical form [8]:

$$I\left(C_1,C_2,C_3,C_4,C_5,C_6\right)=\iint_G\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)-T_{actual}\right)^2 dxdy \rightarrow \min . \tag{1}$$

The partial differential equation that describes the process of heat propagation has the form:

$$\begin{gathered}\rho\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)\right)C\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)\right)\frac{\partial T}{\partial t}= \\ =\frac{\partial}{\partial x}\left(a\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)\right)\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(a\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)\right)\frac{\partial T}{\partial y}\right).\end{gathered} \tag{2}$$

The calculation area in (2) is a rectangular area, which can be written as $[0;A]\times[0;B]$, where A, B – dimensions of the heating area of the furnace. The process described by equation (2) has initial, boundary and internal conditions.

$$\begin{gathered}\left.\frac{\partial T}{\partial x}\right|_{(0;y)}=\left.\frac{\partial T}{\partial x}\right|_{(A;y)}=0, \\ T\left(x,0,C_1,C_2,C_3,C_4,C_5,C_6\right)=T_{Up},\ T\left(x,B,C_1,C_2,C_3,C_4,C_5,C_6\right)=T_{Down}.\end{gathered} \tag{3}$$

The first two equalities in (3), which set the zero values of the derivative, indicate the thermal insulation of the furnace on its two opposite walls. There are no heaters on these walls. The internal conditions for (2) are the temperatures that are supplied to the point electric heaters of the furnace. They can be given as:

$$\begin{gathered}T\left(x_1,y_1\right)=C_1,\ T\left(x_2,y_2\right)=C_2,\ T\left(x_3,y_3\right)=C_3, \\ T\left(x_4,y_4\right)=C_4,\ T\left(x_5,y_5\right)=C_5,\ T\left(x_6,y_6\right)=C_6.\end{gathered} \tag{4}$$

To solve such a problem in this mathematical formulation, it is necessary to have sufficiently effective methods for finding numerical solutions to second-order elliptic-type mathematical physics equations, as well as high-speed optimization methods to accelerate the search for optimal modes in heat and mass transfer processes. The next part of this article contains a description of these methods.

4. Discretization of the nonlinear equation describing the process of heat transfer in a furnace

Equation (2) will be considered in its full form. We will write a discrete representation for it, using the finite difference method for this. The first-order derivatives in spatial coordinates for any time instant, using the central difference scheme, look like [13–15]:

$$\left.\frac{\partial T}{\partial x}\right|_{(i,j)} = \frac{T_{i+0.5,j} - T_{i-0.5,j}}{\Delta x}, \left.\frac{\partial T}{\partial y}\right|_{(i,j)} = \frac{T_{i,j+0.5} - T_{i,j-0.5}}{\Delta y}. \tag{5}$$

Taking into account (5), the expressions for the left-hand side of equation (2) are as follows:

$$\begin{aligned} \left.\left[a\big(T(x,y,t)\big)\frac{\partial T}{\partial x}\right]\right|_{(i,j)} &= a\big(T_{i,j}\big)\frac{T_{i+0.5,j} - T_{i-0.5,j}}{\Delta x} = a_{i,j}\frac{T_{i+0.5,j} - T_{i-0.5,j}}{\Delta x}, \\ \left.\left[a\big(T(x,y,t)\big)\frac{\partial T}{\partial y}\right]\right|_{(i,j)} &= a\big(T_{i,j}\big)\frac{T_{i,j+0.5} - T_{i,j-0.5}}{\Delta y} = a_{i,j}\frac{T_{i,j+0.5} - T_{i,j-0.5}}{\Delta y}. \end{aligned} \tag{6}$$

Using the notations (6), we can write down the difference scheme for the terms of the left-hand side of equation (2). We will have:

$$\begin{aligned} \left.\left[\frac{\partial}{\partial x}\left(a\big(T(x,y,t)\big)\frac{\partial T}{\partial x}\right)\right]\right|_{(i,j)} &= \frac{a_{i+0.5,j}\dfrac{T_{i+1,j} - T_{i,j}}{\Delta x} - a_{i-0.5,j}\dfrac{T_{i,j} - T_{i-1,j}}{\Delta x}}{\Delta x} = \\ &= a_{i+0.5,j}\frac{T_{i+1,j} - T_{i,j}}{\Delta x^2} - a_{i-0.5,j}\frac{T_{i,j} - T_{i-1,j}}{\Delta x^2}, \\ \left.\left[\frac{\partial}{\partial y}\left(a\big(T(x,y,t)\big)\frac{\partial T}{\partial y}\right)\right]\right|_{(i,j)} &= a_{i,j+0.5}\frac{T_{i,j+1} - T_{i,j}}{\Delta y^2} - a_{i,j-0.5}\frac{T_{i,j} - T_{i,j-1}}{\Delta y^2}. \end{aligned} \tag{7}$$

Taking into account (7), we can write down the classical implicit difference scheme for equation (2). It will take the form:

$$\begin{aligned} \rho_{i,j}^{(k+1)}C_{i,j}^{(k+1)}\frac{T_{i,j}^{(k+1)} - T_{i,j}^{(k)}}{\Delta\tau} &= a_{i+0.5,j}^{(k+1)}\frac{T_{i+1,j}^{(k+1)} - T_{i,j}^{(k+1)}}{\Delta x^2} - a_{i-0.5,j}^{(k+1)}\frac{T_{i,j}^{(k+1)} - T_{i-1,j}^{(k+1)}}{\Delta x^2} + \\ &+ a_{i,j+0.5}^{(k+1)}\frac{T_{i,j+1}^{(k+1)} - T_{i,j}^{(k+1)}}{\Delta y^2} - a_{i,j-0.5}^{(k+1)}\frac{T_{i,j}^{(k+1)} - T_{i,j-1}^{(k+1)}}{\Delta y^2}. \end{aligned} \tag{8}$$

It should be noted that in (8) a 5-point difference scheme is used. This difference scheme has a significant drawback. This drawback is manifested in the fact that when finding four values on a new time layer, data on one point from the previous time layer are used. The difference scheme is stable, but does not provide the necessary accuracy of calculations due to damping. To increase the accuracy of calculations, a high-precision scheme is used. It is based on the Crank-Nicholson difference scheme:

$$\rho_{i,j}^{(k+1)} C_{i,j}^{(k+1)} \frac{T_{i,j}^{(k+1)} - T_{i,j}^{(k)}}{\Delta \tau} = \frac{1}{2} \begin{pmatrix} a_{i+0.5,j}^{(k+1)} \frac{T_{i+1,j}^{(k+1)} - T_{i,j}^{(k+1)}}{\Delta x^2} - a_{i-0.5,j}^{(k+1)} \frac{T_{i,j}^{(k+1)} - T_{i-1,j}^{(k+1)}}{\Delta x^2} + \\ + a_{i,j+0.5}^{(k+1)} \frac{T_{i,j+1}^{(k+1)} - T_{i,j}^{(k+1)}}{\Delta y^2} - a_{i,j-0.5}^{(k+1)} \frac{T_{i,j}^{(k+1)} - T_{i,j-1}^{(k+1)}}{\Delta y^2} + \\ + a_{i+0.5,j}^{(k)} \frac{T_{i+1,j}^{(k)} - T_{i,j}^{(k)}}{\Delta x^2} - a_{i-0.5,j}^{(k)} \frac{T_{i,j}^{(k)} - T_{i-1,j}^{(k)}}{\Delta x^2} + \\ + a_{i,j+0.5}^{(k)} \frac{T_{i,j+1}^{(k)} - T_{i,j}^{(k)}}{\Delta y^2} - a_{i,j-0.5}^{(k)} \frac{T_{i,j}^{(k)} - T_{i,j-1}^{(k)}}{\Delta y^2} \end{pmatrix}. \quad (9)$$

It can be seen from equation (9) that it contains factors of the form $a_{i,\pm 0.5,j}$ and $a_{i,j\pm 0.5}$. These factors, as an option, can be approximately replaced by the following formulas:

$$\begin{aligned} a_{i+0.5,j}^{(k+1)} &\approx \frac{1}{2}\left(a_{i+1,j}^{(k+1)} + a_{i,j}^{(k+1)}\right); \quad a_{i-0.5,j}^{(k+1)} \approx \frac{1}{2}\left(a_{i-1,j}^{(k+1)} + a_{i,j}^{(k+1)}\right); \\ a_{i,j-0.5}^{(k+1)} &\approx \frac{1}{2}\left(a_{i,j-1}^{(k+1)} + a_{i,j}^{(k+1)}\right); \quad a_{i,j+1}^{(k+1)} \approx \frac{1}{2}\left(a_{i,j+1}^{(k+1)} + a_{i,j}^{(k+1)}\right). \end{aligned} \quad (10)$$

After such a replacement in (10), we solve the posed direct nonlinear direct heat and mass transfer problem using a difference scheme containing 8 points: 4 on the new (searched layer) and 4 on the old (known layer). But the resulting system of equations is nonlinear. For its implementation, we can use Newton linearization with the subsequent application of classical iterative methods for solving linear equations (for example, the conjugate or biconjugate gradient method). Let us proceed to the process of linearization of the terms of the nonlinear heat and mass transfer equation. To perform the procedure for linearization of functions, we take into account:

$$\left\| T_{i,j}^{(m+1)} - T_{i,j}^{(m)} \right\| < \varepsilon. \quad (11)$$

Then we will have

$$a_{i,j}^{(m+1)} \approx a_{i,j}^{(m)} + a'^{(m)}_{i,j} \left(T_{i,j}^{(m+1)} - T_{i,j}^{(m)} \right). \quad (12)$$

Let us assume that we need to find the temperature distribution at time (k+1). The procedure for obtaining this layer will be performed iteratively. To obtain this temperature distribution at layer (k+1), we use the iterative process (9) based on (11), taking into account (10). As a result, we obtain the following iterative formula:

$$\frac{T_{i,j}^{(m+1)}-T_{i,j}^{(k)}}{\Delta\tau}=\frac{1}{4\rho_{i,j}^{(m)}C_{i,j}^{(m)}}\times\left(\begin{array}{c}\left(a_{i+1,j}^{(m)}+a_{i,j}^{(m)}\right)\frac{T_{i+1,j}^{(m+1)}-T_{i,j}^{(m+1)}}{\Delta x^2}-\left(a_{i-1,j}^{(m)}+a_{i,j}^{(m)}\right)\frac{T_{i,j}^{(m+1)}-T_{i-1,j}^{(m+1)}}{\Delta x^2}+\\+\left(a_{i,j+1}^{(m)}+a_{i,j}^{(m)}\right)\frac{T_{i,j+1}^{(m+1)}-T_{i,j}^{(m+1)}}{\Delta y^2}-\left(a_{i,j-1}^{(m)}+a_{i,j}^{(m)}\right)\frac{T_{i,j}^{(m+1)}-T_{i,j-1}^{(m+1)}}{\Delta y^2}+\\+\left(a_{i+1,j}^{(k)}+a_{i,j}^{(k)}\right)\frac{T_{i+1,j}^{(k)}-T_{i,j}^{(k)}}{\Delta x^2}-\left(a_{i-1,j}^{(k)}+a_{i,j}^{(k)}\right)\frac{T_{i,j}^{(k)}-T_{i-1,j}^{(k)}}{\Delta x^2}+\\+\left(a_{i,j+1}^{(k)}+a_{i,j}^{(k)}\right)\frac{T_{i,j+1}^{(k)}-T_{i,j}^{(k)}}{\Delta y^2}-\left(a_{i,j-1}^{(k)}+a_{i,j}^{(k)}\right)\frac{T_{i,j}^{(k)}-T_{i,j-1}^{(k)}}{\Delta y^2}\end{array}\right). \quad (13)$$

After condition (11) is satisfied, the solution (13) is obtained $T_{i,j}^{(m+1)}$ accepted as wanted $T_{i,j}^{(k+1)}$ The beginning of the iterative process is provided by the initial condition for equation (2). That is, for the desired values on the new time layer, the temperature distribution from the previous time layer is taken (the values are already known) –). The$T_{i,j}^{(k)}$ above technique is not a direct linearization, but this approach is often used when solving nonlinear equations in mathematical physics in general.

Let's return to equation (2):

$$\rho(T)C(T)\frac{\partial T}{\partial\tau}=\frac{\partial}{\partial x}\left(a(T)\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(a(T)\frac{\partial T}{\partial y}\right).$$

The Crank-Nicholson difference scheme for this equation has the form:

$$\begin{gathered}\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)+\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)}{2}\frac{T_{i,j}^{k+1}-T_{i,j}^{k}}{\partial\tau}=\\=0.5\left(\frac{a\left(T_{i+1,j}^{k+1}\right)+a\left(T_{i,j}^{k+1}\right)}{2}\frac{T_{i+1,j}^{k+1}-T_{i,j}^{k+1}}{hx^2}-\frac{a\left(T_{i,j}^{k+1}\right)+a\left(T_{i-1,j}^{k+1}\right)}{2}\frac{T_{i,j}^{k+1}-T_{i-1,j}^{k+1}}{hx^2}\right)+\\+0.5\left(\frac{a\left(T_{i+1,j}^{k}\right)+a\left(T_{i,j}^{k}\right)}{2}\frac{T_{i+1,j}^{k}-T_{i,j}^{k}}{hx^2}-\frac{a\left(T_{i,j}^{k}\right)+a\left(T_{i-1,j}^{k}\right)}{2}\frac{T_{i,j}^{k}-T_{i-1,j}^{k}}{hx^2}\right)+\\+0.5\left(\frac{a\left(T_{i,j+1}^{k+1}\right)+a\left(T_{i,j}^{k+1}\right)}{2}\frac{T_{i,j+1}^{k+1}-T_{i,j}^{k+1}}{hy^2}-\frac{a\left(T_{i,j}^{k+1}\right)+a\left(T_{i,j-1}^{k+1}\right)}{2}\frac{T_{i,j}^{k+1}-T_{i,j-1}^{k+1}}{hy^2}\right)+\\+0.5\left(\frac{a\left(T_{i,j+1}^{k}\right)+a\left(T_{i,j}^{k}\right)}{2}\frac{T_{i,j+1}^{k}-T_{i,j}^{k}}{hy^2}-\frac{a\left(T_{i,j}^{k}\right)+a\left(T_{i,j-1}^{k}\right)}{2}\frac{T_{i,j}^{k}-T_{i,j-1}^{k}}{hy^2}\right).\end{gathered} \quad (14)$$

The left-hand side of equation (14) can be rewritten as:

$$\begin{gathered}\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)+\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)}{2}\frac{T_{i,j}^{k+1}-T_{i,j}^{k}}{h\tau}=\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)T_{i,j}^{k+1}+\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)T_{i,j}^{k+1}}{2h\tau}-\\-\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)T_{i,j}^{k}+\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)T_{i,j}^{k}}{2h\tau}=\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)T_{i,j}^{k+1}}{2h\tau}+\frac{\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)}{2h\tau}T_{i,j}^{k+1}-\\-\frac{\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)T_{i,j}^{k}}{2h\tau}-\frac{\rho\left(T_{i,j}^{k}\right)C\left(T_{i,j}^{k}\right)}{2h\tau}T_{i,j}^{k}.\end{gathered} \quad (15)$$

In (15) it is necessary to perform linearization for the first and third terms of the right-hand side. Linearization by Newton's method for any function $f(x)$ is carried out according to the following formula:

$$f\left(x^{k+1}\right)=f\left(x^{k}\right)+\left(x^{k+1}-x^{k+1}\right)\frac{df}{dx}\left(x^{k}\right). \tag{16}$$

Let $\rho(T)=\Sigma a_i^{\rho} T^i$ and $C(T)=\Sigma a_i^{C} T^i$. Then we will have:

$$\begin{gathered}
\rho_{i,j}^{k+1}C_{i,j}^{k+1}T_{i,j}^{k+1}=\rho_{i,j}^{k}C_{i,j}^{k}T_{i,j}^{k}+\left(T_{i,j}^{k+1}-T_{i,j}^{k}\right)\left(\left(\rho_{i,j}'^{k}C_{i,j}^{k}+\rho_{i,j}^{k}C_{i,j}'^{k}\right)T_{i,j}^{k}+\rho_{i,j}^{k}C_{i,j}^{k}\right),\\
a_{i+1,j}^{k+1}T_{i+1,j}^{k+1}=a_{i+1,j}^{k}T_{i+1,j}^{k}+\left(T_{i+1,j}^{k+1}-T_{i+1,j}^{k}\right)\left(a_{i+1,j}^{k+1}+a'^{k+1}_{i+1,j}\right),\\
\left(a_{i+1,j}^{k+1}+a_{i,j}^{k+1}\right)T_{i,j}^{k+1}=\left(a_{i+1,j}^{k}+a_{i,j}^{k}\right)T_{i,j}^{k}+\left(T_{i,j}^{k+1}-T_{i,j}^{k}\right)\left(a_{i+1,j}^{k+1}+a_{i,j}^{k+1}+a'^{k+1}_{i+1,j}+a'^{k+1}_{i,j}\right)
\end{gathered} \tag{17}$$

Taking into account (17), we obtain an expression for the first nonlinear term on the right-hand side of equation (15).

$$\begin{gathered}
\rho\left(T_{i,j}^{k+1}\right)C\left(T_{i,j}^{k+1}\right)T_{i,j}^{k+1}=\left(\sum_{l=0} a_l^{\rho}\left(T_{i,j}^{k+1}\right)^{l}\right)\left(\sum_{m=0} a_m^{\rho}\left(T_{i,j}^{k+1}\right)^{m}\right)T_{i,j}^{k+1}=\\
=\left(\sum_{l=0}^{n} a_l^{\rho}\left(T_{i,j}^{k}\right)^{l}\right)\left(\sum_{m=0}^{n} a_m^{\rho}\left(T_{i,j}^{k}\right)^{m}\right)T_{i,j}^{k}+\left(T_{i,j}^{k+1}-T_{i,j}^{k}\right)\times\\
\times\left[\left(\sum_{l=1}^{n} l a_l^{\rho}\left(T_{i,j}^{k}\right)^{l-1}\right)\left(\sum_{m=0}^{n} a_m^{\rho}\left(T_{i,j}^{k}\right)^{m}\right)T_{i,j}^{k}+\left(\sum_{l=0}^{n} a_l^{\rho}\left(T_{i,j}^{k}\right)^{l}\right)\left(\sum_{m=1}^{n} m a_m^{\rho}\left(T_{i,j}^{k}\right)^{m-1}\right)T_{i,j}^{k}+\right.\\
\left.+\left(\sum_{l=0}^{n} a_l^{\rho}\left(T_{i,j}^{k}\right)^{l}\right)\left(\sum_{m=0}^{n} a_m^{\rho}\left(T_{i,j}^{k}\right)^{m}\right)T_{i,j}^{k}\right].
\end{gathered} \tag{18}$$

Similarly to (18), linearization is performed for any function with the aim of constructing an efficient iterative process for solving equation (2).

5. Construction of optimization methods and algorithms

In the study of inverse heat and mass transfer problems, an important place is occupied by optimization methods aimed at restoring unknown parameters or boundary conditions from available experimental or calculated data. The most common approach is to reduce the identification problem to the problem of minimizing the quadratic residual functional, which characterizes the difference between the calculated and experimentally measured temperature field. Such functionals have, as a rule, a strictly convex structure, which makes the use of deterministic optimization methods effective.

Classical deterministic methods include gradient methods (the method of steepest descent, the gradient design method), which are based on the use of the first derivative of the functional. Their effectiveness in heat and mass transfer problems is due to the relative simplicity of calculating derivatives, in particular using sensitivity methods or the adjoint approach. However, such methods are often characterized by a slow convergence rate in conditions of poorly conditioned problems.

Second-order methods, in particular Newton's method and quasi-Newton approaches, are more efficient. They involve the use of information about the Hessian matrix of the functional or its approximation. For quadratic functionals, these methods guarantee quadratic convergence and have proven themselves particularly well in restoring the parameters of thermophysical processes.

The necessary condition for the existence of a minimum of the functional (1) has the classical form:

$$\begin{cases} \frac{\partial I}{\partial C_1}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0, \\ \frac{\partial I}{\partial C_2}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_2}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0, \\ \frac{\partial I}{\partial C_3}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0, \\ \frac{\partial I}{\partial C_4}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0, \\ \frac{\partial I}{\partial C_5}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0, \\ \frac{\partial I}{\partial C_6}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)=0. \end{cases} \tag{19}$$

It is obvious that all derivatives given in (19) must be given numerically based on approximation methods, for example, using the left difference scheme:

$$I'_{C_1}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)\approx$$
$$\approx\frac{1}{\Delta C_1}\left[\begin{array}{l}\iint\limits_G \left(T(x,y,C_1+\Delta C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy- \\ -\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\end{array}\right],$$

or using the left difference scheme:

$$I'_{C_1}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)\approx$$
$$\approx\frac{1}{\Delta C_1}\left[\begin{array}{l}\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy- \\ -\iint\limits_G \left(T(x,y,C_1-\Delta C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\end{array}\right].$$

The central difference scheme for (1) can be written as follows:

$$I'_{C_1}(C_1,C_2,C_3,C_4,C_5,C_6)=\frac{\partial}{\partial C_1}\left(\iint\limits_G \left(T(x,y,C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\right)\approx$$
$$\approx\frac{1}{2\Delta C_1}\left[\begin{array}{l}\iint\limits_G \left(T(x,y,C_1+\Delta C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy- \\ -\iint\limits_G \left(T(x,y,C_1-\Delta C_1,C_2,C_3,C_4,C_5,C_6)-T_{actual}\right)^2 dxdy\end{array}\right].$$

If second-order methods are used, for example, Newton's method and its modifications, it is necessary to use the Hessian matrix to approximate the second derivatives. Here it is better to use the central cutting scheme to approximate the second derivatives, in particular, the mixed second-order derivatives will have the following form:

$$\frac{\partial}{\partial C_j}\left(\frac{\partial}{\partial C_i}\left(\iint_G \left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)-T_{actual}\right)^2 dxdy\right)\right)=$$
$$=\frac{\partial}{\partial C_j}\left(\iint_G \frac{\partial}{\partial C_i}\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)-T_{actual}\right)^2 dxdy\right)=$$
$$=\iint_G \frac{\partial}{\partial C_j}\left(2\left(T-T_{actual}\right)\cdot\frac{\partial T}{\partial C_i}\right)dxdy=2\iint_G \frac{\partial}{\partial C_j}\left(\left(T-T_{actual}\right)\cdot\frac{\partial T}{\partial C_i}\right)dxdy=$$
$$=2\iint_G\left(\frac{\partial\left(T-T_{actual}\right)}{\partial C_j}\frac{\partial T}{\partial C_i}+\left(T-T_{actual}\right)\cdot\frac{\partial^2 T}{\partial C_i\partial C_j}\right)dxdy=$$
$$=2\iint_G\left(\frac{\partial T}{\partial C_j}\cdot\frac{\partial T}{\partial C_i}+\left(T-T_{actual}\right)\cdot\frac{\partial^2 T}{\partial C_i\partial C_j}\right)dxdy.$$

Similarly, we obtain expressions for specifying the second-order derivatives of the functional (1) with respect to the same variable:

$$\frac{\partial}{\partial C_i}\left(\frac{\partial}{\partial C_i}\left(\iint_G \left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)-T_{actual}\right)^2 dxdy\right)\right)=$$
$$=\frac{\partial}{\partial C_i}\left(\iint_G \frac{\partial}{\partial C_i}\left(T\left(x,y,C_1,C_2,C_3,C_4,C_5,C_6\right)-T_{actual}\right)^2 dxdy\right)=$$
$$=\iint_G \frac{\partial}{\partial C_i}\left(2\left(T-T_{actual}\right)\cdot\frac{\partial T}{\partial C_i}\right)dxdy=2\iint_G \frac{\partial}{\partial C_i}\left(\left(T-T_{actual}\right)\cdot\frac{\partial T}{\partial C_i}\right)dxdy=$$
$$=2\iint_G\left(\frac{\partial\left(T-T_{actual}\right)}{\partial C_i}\frac{\partial T}{\partial C_i}+\left(T-T_{actual}\right)\cdot\frac{\partial^2 T}{\partial C_i^2}\right)dxdy=$$
$$=2\iint_G\left(\left(\frac{\partial T}{\partial C_1}\right)^2+\left(T-T_{actual}\right)\cdot\frac{\partial^2 T}{\partial C_1^2}\right)dxdy.$$

In the last expression:

$$\frac{\partial^2 T}{\partial C_1^2}\approx\frac{T\left(C_1+\Delta C_1\right)-2T+T\left(C_1-\Delta C_1\right)}{\Delta C_1^2},$$
$$\frac{\partial^2 T}{\partial C_1\partial C_j}\approx\frac{1}{\Delta C_1^2}\begin{bmatrix}T\left(C_i+\Delta C_i,C_j+\Delta C_j\right)+T\left(C_i-\Delta C_i,C_j-\Delta C_j\right)-\\-T\left(C_i-\Delta C_i,C_j+\Delta C_j\right)-T\left(C_i-\Delta C_i,C_j+\Delta C_j\right)\end{bmatrix}.$$

To obtain modifications of the methods, it is necessary to use the multi-grid principle, which allows obtaining faster solutions without loss of accuracy.

In practical applications of inverse heat and mass transfer problems, iterative deterministic algorithms with combined strategies, which combine gradient information with regularization approaches, have become widespread. Such algorithms are reliable, have guaranteed convergence and relatively high speed of solving problems.

6. Modified multigrid method for solving direct problems as components of inverse heat and mass transfer problems

When solving inverse heat and mass transfer problems, it is necessary to solve a significant number of direct heat and mass transfer problems. Therefore, the proposed method will be applied specifically to solving direct heat and mass transfer problems, since they are the basis for solving inverse heat and mass transfer problems. For the sake of simplicity, let us consider a certain two-dimensional domain in which the inverse heat and mass transfer problems are solved. The solution of a two-dimensional problem is represented as a table of values of the desired function at each point of a certain grid into which the computational domain is divided. Let the differential equation be solved in partial derivatives by the difference method $L(y)=0$. A system of linear algebraic equations is solved by an iterative method. The main idea of the multigrid method is as follows. Let the initial condition for solving systems of equations be in the form

$$T = u_0 + \sum\sum \sin\left(2^{k_1}\pi x\right)\sin\left(2^{k_2}\pi y\right)$$

Here T is the exact solution. Then the iterative procedure for finding a numerical solution is considered as a process of error reduction.

$$err = T - u_0 = \sum\sum \sin\left(2^{k_1}\pi x\right)\sin\left(2^{k_2}\pi y\right)$$

It is obvious that the components with a half-period equal to the grid step are destroyed most quickly, the slowest of all are the long-wave components with a half-period equal to the length of the entire calculation area. From solving the algebraic system of equations with respect to the values of the desired quantity, it is necessary to proceed to the system of equations with respect to the error.

Let $A_h T_h = b_h$ is a system of equations built on a grid with a step h, T_h is its exact solution. It is clear that the exact solution of this system of equations can be represented in the form

$$T_h = err_h^k + u_h^k$$

where u_h^k is the result of the kth step of the iterative method and err_h^k is the error of this step, $r_h^k = b_h - A_h u_h^k$ its residual, then, substituting into the ratio $A_h T_h = b_h$ expression $T_h = err_h^k + u_h^k$, we get $A_h(err_h^k + u_h^k) = b_h$ or ,$A_h err^k = b_h - A_h u_h^k = r_h^k$ that is, the equation for the error. Solving this equation, we find err_h^k, and therefore . Th$T_h = err_h^k + u_h^k$e next step is to choose the initial conditions for solving the system of equations. To calculate the error, we will use the system $A_h(err_h^0) = r_h^0$, where $r_h^0 = b_h - A_h u_h^0$, a u_h^0 is the initial condition. The right-hand side of the system must be related to the original problem. Therefore, the algorithm looks as follows. On a dense grid, we build a system of difference equations and perform several iterations. Based on the obtained result, we build a system of equations for the error. To suppress the long-wave components of the error, we project the system onto a sparse grid, solve it, and obtain a solution without the long-wave component of the error. We project the result onto a dense grid and solve the problem finally. After finding the error, we add it to the initial conditions and obtain a solution to the original problem. This method was used when testing the following stationary direct heat and mass transfer problems.

Problem 1. Find a numerical solution to the following boundary value problem:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 1, (x; y) \in [0;1]^2, T|_\Gamma = 0, \tag{20}$$

where G is the boundary of the computational domain. The numerical solution of problem (6) is given in Figure 3:

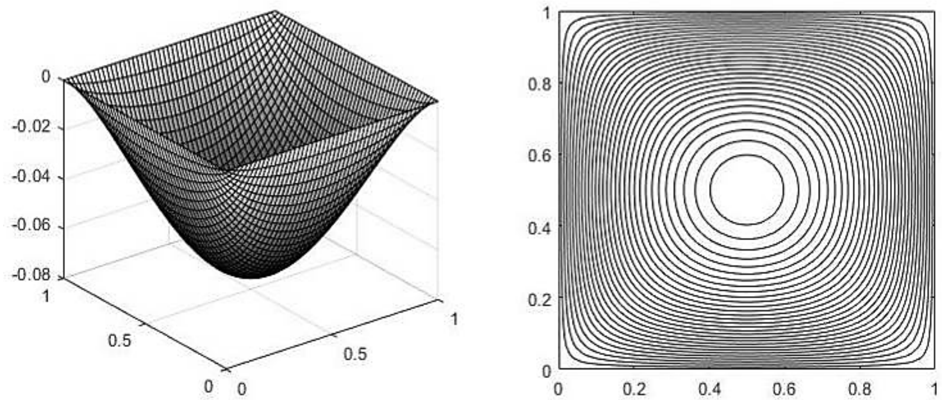

Figure 3: Numerical solution of problem (20): left – surface; right – contour lines

Problem 2. Find a numerical solution to the following boundary value problem:

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=x^2+y^2,(x;y)\in[0;2]^2,$$
$$T(0;y)=1,\ \partial T/\partial x(2;y)=0,\ T(x;0)=-2,\ \partial T/\partial y(x;2)=0. \tag{21}$$

The numerical solution of problem (7) is shown in Figure 4:

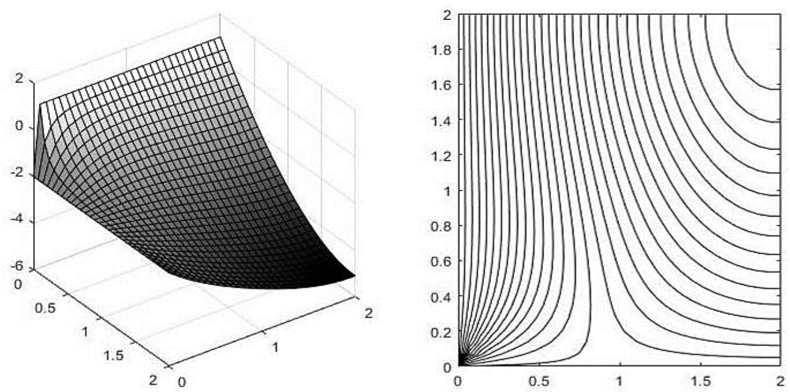

Figure 4: Numerical solution of problem (21): left – surface; right – contour lines

Below (Table 1) are the results of the multi-grid method based on the V-cycle according to the criterion of the number of iterations.

Table 1
Results of applying the V-cycle to solve problems (20) and (21). Calculation accuracy 1.0E-07. Grid 128x128 nodes. Number of calculation grids – 7

Task number	Number of iterations to obtain a solution to the problem using the Gauss-Seidel method	Number of iterations to obtain a solution to the problem by the multi-grid method using the Gauss-Seidel method
(20)	14534 iterations	1374 iterations
(21)	105422 iterations	12587 iterations

Based on the results obtained, it can be stated that the application of multigrid methods to find a numerical solution of nonlinear inverse problems is a rational approach. Using multigrid methods, a numerical solution to the problem can be obtained tens of times faster compared to the time of solving the same problem by classical methods on the same grid. As already mentioned, the multigrid method is used when solving direct heat conduction problems, which are not used once to solve one inverse heat conduction problem. Below in Table 2, the main results of modeling with and without the multigrid method described in the work are presented.

Table 2
The result of finding a numerical solution to problem (5) using the multi-grid method. Calculation accuracy 1.0E-07. Final grid 128x128 nodes. Number of calculation grids – 5

Grid Dimension	Number of Iterations to Solve a Problem Using the Gauss-Seidel Method	Number of Iterations to Solve a Problem Using classic Multigrid Method	Number of Iterations to Solve a Problem Using the Multigrid Method Using the Gauss-Seidel Method
64x64	7588156 iterations	236367 iterations	113212 iterations
128x128	57568581 iterations	984512 iterations	622242 iterations
256x256	230362607 iterations	3535545 iterations	1842324 iterations

Table 2 shows that the total number of iterations when using the modified multigrid method is reduced by a factor of 2–4. This is a significant result, considering that such problems as (20) and (21) are used to solve a problem of type (1) with constraints (2) and boundary and internal conditions (3) and (40), respectively.

Conclusion

The article builds a mathematical model for solving inverse heat and mass transfer problems based on the minimization of a quadratic functional that takes into account the differences between the actual and model temperature fields. To find optimal modes, the basic equation that mathematically describes the process of heat propagation in an industrial / muffle furnace is discretized. A modification of the method for solving the main classes of inverse heat and mass transfer problems using multi-grid methods based on the already known V-cycle is proposed. The method is tested in comparison with the classical multi-grid V-cycle. The results obtained confirm the effectiveness of the proposed approach for modeling and analyzing heat engineering processes, which creates the prerequisites for further use of the developed methods in applied problems of energy and industrial heat and mass transfer. The obtained modification of the multi-grid method speeds up calculations for solving one direct problem by 2–4 times. This means that in practice, the number of calculations when solving a single inverse problem can be up to 10 times.

Declaration on Generative AI

The author(s) have not employed any Generative AI tools.

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