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NUMERICAL SOLUTION OF ONE INVERSE PROBLEM FOR A DIFFUSION MODEL OF A CHEMICAL-TECHNOLOGICAL PROCESS

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Abstract. *A chemical-technological process taking place in a chemical reactor with a chemical reaction of the second order is considered. A one-dimensional one-parameter diffusion model of the hydrodynamic flow in the reactor is proposed for the mathematical description of this process. Within the framework of the proposed model, the inverse problem is posed to determine the concentration of the selected reagent in the incoming flow, ensuring the implementation of a predetermined hydrodynamic regime at the reactor outlet. A discrete analogue of the inverse problem is constructed and the resulting difference problem is presented as a variational problem with local regularization. A special representation is proposed for the numerical solution of the variational problem. As a result, an explicit formula is obtained for determining the approximate concentration of the selected reagent in the incoming stream. The effectiveness of the proposed method is illustrated by numerical calculations for model problems*

Keywords: chemical reactor, second-order chemical reaction, one-parameter diffusion model, boundary inverse problem, local regularization method

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1. Introduction

It is known that the central element in any chemical-technological system is a chemical reactor, in which interrelated hydrodynamic, thermal, and diffusion processes are carried out, with the help of which conditions are created for the chemical transformation of a

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substance, i.e. a chemical reaction [8], [9], [12]. However, the kinetics of the chemical-technological process is mainly determined by the hydrodynamic regularity of the flow of the reaction medium in the reactor. In chemical technology, a large number of different types and designs of chemical reactors are used, which are classified according to a number of characteristics.

Currently, the most common classification of chemical reactors is based on the hydrodynamic mode of movement of the reaction medium in reactors. To describe various hydrodynamic flows in chemical reactors, models are used: ideal mixing; ideal displacement; diffusion models; cell models; combined models [5], [7], [16], [18]. One-parameter and two-parameter diffusion models are mainly used to describe most of the real hydrodynamic flows in chemical reactors. According to the one-parameter diffusion model, the mixing of reagents in reactors occurs only in the longitudinal direction. And according to the two-parameter diffusion model, longitudinal and radial mixing of reagents occurs simultaneously in the hydrodynamic flow. Diffusion models accurately reflect the structure of hydrodynamic flows in many real reactors: film, spray, bubbling columns, extractors, etc. [8], [12].

When modeling the processes occurring in chemical reactors, an important step is considered to be the provision of appropriate mathematical models with the necessary quantitative information, i.e. the determination of the parameters of mathematical models. Usually, the parameters of a mathematical model quantitatively and unambiguously describe certain characteristics of a chemical-technological process.

The determination of the parameters of mathematical models is a defining moment, on which the adequacy of the constructed mathematical model and the effectiveness of the control of the chemical process using the constructed model largely depend. In this regard, the creation of one or another hydrodynamic mode of operation of reactors using controlling the parameters of mathematical models of chemical and technological processes is of great practical importance. In this paper, the problem of creating a predetermined reactor operation mode using a controlled parameter of a one-parameter diffusion model of hydrodynamic flow is investigated.

2. Problem Statement

Suppose that a chemical reactor, which is a tubular apparatus, continuously receives a reaction stream. The incoming flow moves only in one direction along the length of the reactor and a second-order chemical reaction takes place with the participation of the reagent under study in the flow. It is assumed that the change in the concentration of the selected reagent in the reactor occurs due to its transfer by the reaction medium (convective transfer) in the direction coinciding with the direction of the general flow and as a result of its transfer by diffusion (diffusion transfer). In the reactor, only longitudinal mixing of the reagent under study in the reaction mixture takes place and the values of the parameters of the reaction mixture along the reactor cross-section are the same. The reactor operates in an isothermal mode and, by the laws of the chemical reaction, a certain distribution of concentrations of reagents involved in the reaction is established along the length of the reactor. To describe the process occurring in this chemical reactor,

we use a one-dimensional, one-parameter diffusion model of the hydrodynamic flow of the reaction medium, taking into account the flow of a second-order chemical reaction

$$\frac{\partial\psi(x,t)}{\partial t}+\nu(t)\frac{\partial\psi(x,t)}{\partial x}+k\psi^2(x,t)=d\frac{\partial^2\psi(x,t)}{\partial x^2},0<x<l,\quad 0<t\leq T, \tag{1}$$

where $\psi(x,t)$ is the concentration of the reagent under study, $v(t)$– the rate of the reaction flow in the reactor, d– the coefficient of turbulent diffusion, k – the rate constant of the chemical reaction, l– the length of the chemical reactor, x– the coordinate along which the reaction flow moves, t– time.

Assume that at the initial moment, the distribution of the reagent concentration along the length of the reactor is known, i.e., for equation (1) we have the following initial condition.

$$\psi(x,0)=\phi(x),0\leq x\leq l. \tag{2}$$

The boundary conditions at the reactor inlet and outlet are formulated according to the Danckverts condition: the sum of the flows of matter approaching the reactor boundary should be equal to the flow of matter departing from the boundary [2], [7]. As a result, we will have.

$$\nu(t)\psi_e(t)+d\frac{\partial\psi(0,t)}{\partial x}=v(t)\psi(0,t), \tag{3}$$

$$\frac{\partial\psi(l,t)}{\partial x}=0, \tag{4}$$

where $\psi_e(t)$ is the concentration of the selected reagent in the incoming stream. If we set the functions $v(t)$, $\psi_e(t)$, $\phi(x)$ and values of the constant parameters d, k, then by solving the problem (1)-(4), we can find the function $\psi(x,t)$, i.e. the distribution of the reagent concentration along the length of the reactor. However, for chemical-technological systems, the task of determining the hydrodynamic condition at the reactor inlet necessary for the implementation of a predetermined hydrodynamic regime at the reactor outlet is important. In this regard, within the framework of model (1)-(4), we set the following task:

determine the concentration of the selected reagent $\psi_e(t)$ in the incoming stream so that the concentration of the reagent at the reactor outlet, along with condition (4), satisfies the additional condition

$$\psi(l,t)=f(t). \tag{5}$$

Thus, the task is to determine the functions $\psi(x,t)$ and $\psi_e(t)$, satisfying equation (1) and conditions (2)-(5). Problem (1)-(5) belongs to the class of boundary inverse problems [1], [6], [15]. The correctness of the formulation of boundary inverse problems and their solutions' existence and uniqueness in various functional classes are investigated in [6], [10], [11], [13], [14]. Numerical methods for solving boundary inverse problems for parabolic equations are considered in many papers [1], [3], [4], [15], [17].

3. Method for Solving the Problem

Assuming the existence of a solution and unambiguous solvability of the boundary inverse problem (1)–(5), we first construct its discrete analog by the method of difference approximation. To this end, we introduce a uniform space-time difference grid

$$\overline{\omega} = \{(x_i, t_j) : x_i = i\Delta x, \quad t_j = j\Delta t, \quad i = 0, 1, 2, ...n, \quad j = 0, 1, 2, ...m\}$$

in a rectangular area $\{0 \le x \le l,\ 0 \le t \le T\}$ with steps $\Delta x = l/n$ and $\Delta t = T/m$.

To obtain a linear difference problem as a discrete analog of the problem (1)–(4), we use explicit-implicit approximations in time. To this end, the convective and diffusion terms in equation (1) are implicitly approximated, and the nonlinear term $k\psi^2(x,t)$, which describes a chemical reaction process, is explicitly approximated in time. As a result, we get a discrete analog of the problem (1)–(5) on the grid $\overline{\omega}$

$$\frac{\psi_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{\psi_i^j - \psi_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 = d\frac{\psi_{i+1}^j - 2\psi_i^j + \psi_{i-1}^j}{\Delta x^2}, \tag{6}$$

$$i = 1,\ 2,\ \ldots n-1,$$

$$v^j \psi_e^j + d\frac{\psi_1^j - \psi_0^j}{\Delta x} = v^j \psi_0^j, \tag{7}$$

$$\frac{\psi_n^j - \psi_{n-1}^j}{\Delta x} = 0, \tag{8}$$

$$\psi_n^j = f^j, \quad j = 1, 2, ..., m, \tag{9}$$

$$\psi_i^0 = \phi_i, \quad i = 0, 2, ..., n, \tag{10}$$

where $\psi_i^j \approx \psi(x_i, t_j)$, $\phi_i = \phi(x_i)$, $f^j = f(t_j)$, $\psi_e^j \approx \psi_e(t_j)$, $v^j = v(t_j)$.

The resulting system of difference equations for each fixed value j, $j = 1, 2, ..., m$ is a system of linear algebraic equations in which the approximate values of the desired functions $\psi(x,t)$ and $\psi_e(t)$ in the nodes of the difference grid act as unknowns, i.e. ψ_i^j, ψ_e^j. The difference problem (6)–(10) is formulated as a variational problem using local regularization [11]. To do this, by (9), we introduce a smoothing functional in the form

$$J(\psi_e^j) = \left[\psi_n^j - f^j\right]^2 + \gamma(\psi_e^j)^2 \to \min \tag{11}$$

where γ– regularization parameter. Thus, the task of determining the concentration of the selected reagent ψ_e^j in the incoming stream is reduced to the task of minimizing the smoothing functional (11) on each time layer $j = 1, 2, ..., m$ when conditions (6)–(8) are met. For the decomposition of the system of difference equations (6)–(8) into mutually independent subsystems, its solution for each fixed value $j = 1, 2, ..., m$ is represented as [9], [12]

$$\psi_i^j = u_i^j + \psi_e^j w_i^j, \quad i = 0, 1, 2, ..., n, \tag{12}$$

where u_i^j, w_i^j and ψ_e^j – unknown variables.

Substituting the ratio (12) into equation (6), we will have

$$\frac{u_i^j + \psi_e^j w_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{u_i^j + \psi_e^j w_i^j - u_{i-1}^j - \psi_e^j w_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 =$$

$$= d\frac{u_{i+1}^j + \psi_e^j w_{i+1}^j - 2u_i^j - 2\psi_e^j w_i^j + u_{i-1}^j + \psi_e^j w_{i-1}^j}{\Delta x^2}$$

or

$$\left[\frac{u_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{u_i^j - u_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 - d\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}\right] +$$

$$+\psi_e^j \left[\frac{w_i^j}{\Delta t} + v^j \frac{w_i^j - w_{i-1}^j}{\Delta x} - d\frac{w_{i+1}^j - 2w_i^j + w_{i-1}^j}{\Delta x^2}\right] = 0.$$

Substituting representation (12) into (7), (8), gives

$$\left[d\frac{u_1^j - u_0^j}{\Delta x} - v^j u_0^j\right] + \psi_e^j \left[v^j + d\frac{w_1^j - w_0^j}{\Delta x} - v^j w_0^j\right] = 0,$$

$$\frac{u_n^j - u_{n-1}^j}{\Delta x} + \psi_e^j \frac{w_n^j - w_{n-1}^j}{\Delta x} = 0.$$

Assume that the auxiliary variables u_i^j, w_i^j are solutions to the following two independent difference problems

$$\frac{u_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{u_i^j - u_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 - d\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2} = 0, \tag{13}$$

$$d\frac{u_1^j - u_0^j}{\Delta x} - v^j u_0^j = 0, \tag{14}$$

$$\frac{u_n^j - u_{n-1}^j}{\Delta x} = 0. \tag{15}$$

$$\frac{w_i^j}{\Delta t} + v^j \frac{w_i^j - w_{i-1}^j}{\Delta x} - d\frac{w_{i+1}^j - 2w_i^j + w_{i-1}^j}{\Delta x^2} = 0, \tag{16}$$

$$v^j + d\frac{w_1^j - w_0^j}{\Delta x} - v^j w_0^j = 0, \tag{17}$$

$$\frac{w_n^j - w_{n-1}^j}{\Delta x} = 0. \tag{18}$$

When using decomposition (12), equations (6) and conditions (7), (8) are executed automatically for any ψ_e^j. The difference problems (13)–(15) and (16)–(18) for each fixed value j, $j = 1, 2, ..., m$ are a system of linear algebraic equations with a tridiagonal matrix and solutions of these systems can be found by the Thomas method [15]. Substituting representation (12) into (11), we will have.

$$J(\psi_e^j) = \left[u_n^j + \psi_e^j w_n^j - f^j\right]^2 + \gamma(\psi_e^j)^2 \to \min.$$

The minimum of this functionality is achieved when the condition is met

$$\left[u_n^j + \psi_e^j w_n^j - f^j\right] w_n^j + \gamma \psi_e^j = 0.$$

From here we obtain a formula for determining the approximate value of the desired function $\psi_e(t)$ at $t = t_j$, i.e. ψ_e^j.

$$\psi_e^j = \frac{w_n^j (f^j - u_n^j)}{(w_n^j)^2 + \gamma}. \tag{19}$$

Thus, a computational algorithm for solving a variational problem with local regularization (6)–(8), (11) by definition ψ_i^j and ψ_e^j, $i = 0, 1, 2, ..., n$, on each time layer j, $j = 1, 2, ..., m$, consists of the following stages:

I. The solutions of two independent difference problems (13)–(15) and (16)–(18) concerning auxiliary variables u_i^j, w_i^j, $i = 0, 1, 2, ..., n$ are determined,

II. The formula (19) determines the approximate value of the desired function $\psi_e(t)$ at $t = t_j$, i.e. ψ_e^j;

III. The values of variables ψ_i^j, $i = 0, 1, 2, ..., n$ are calculated according to the formula (12).

4. Results of Numerical Calculations

To test the operability of the proposed computational algorithm, numerical experiments were carried out for model problems. Numerical experiments were carried out according to the following scheme:

1) for a given function$\psi_e(t)$, the solution of the problem (1)–(4) is determined, i.e. the function $\psi(x, t)$, $0 \le x \le l,\ 0 \le t \le T$,

2) the found dependence $f(t) = \psi(l, t)$ is taken as the exact input data for solving the inverse problem of restoring $\psi_e(t)$.

The first series of calculations was performed using undisturbed input data. In this case, the value of the regularization parameter γ is assumed to be zero. The second series of calculations were carried out when applying one of some function modeling the error of experimental data

$$\tilde{f}(t) = f(t) + \delta \xi(t) f(t)\,,$$

where δ–the error level, $\xi(t)$ is a random variable, modeled using a random number sensor. In this case, the value of the regularization parameter is determined by the residual principle [1], [3].

Numerical experiments were carried out on a space-time difference grid with steps of $\Delta t = 0.5\,s$, $\Delta x = 0,02\,m$ for the following exact values of the desired function $\psi_e(t) = 0.4$; 0.6; $0.85\,m^3/kg$ at $d = 0.5\,m^2/s$, $k = 0,5\,m^3/(kg \cdot s)$, $v(t) = 0,2\,m/s$, $\varphi(x) = 0$, $l = 2\,m$.

The results of numerical experiments conducted with undisturbed and perturbed input data are presented in Table 1; in it t– the time, ψ_e–the exact values of the desired function$\psi_e(t)$, $\bar{\psi}_e$ and $\tilde{\psi}_e$– the calculated values for undisturbed and perturbed input data. To perturb the input data, the following was used as the error level $\delta = 5 \cdot 10^{-4}$.

Table 1. Results of numerical calculations by definition $\psi_e(t)$

t, s	$\psi_e = 0.4\,m^3/kg$		$\psi_e = 0.6\,m^3/kg$		$\psi_e = 0.85\,m^3/kg$	
	$\bar{\psi}_e$	$\tilde{\psi}_e$	$\bar{\psi}_e$	$\tilde{\psi}_e$	$\bar{\psi}_e$	$\tilde{\psi}_e$
10	0.400	0.392	0.600	0.589	0.850	0.836
20	0.400	0.395	0.600	0.594	0.850	0.843
30	0.400	0.390	0.600	0.588	0.850	0.836
40	0.400	0.403	0.600	0.604	0.850	0.855
50	0.400	0.397	0.600	0.596	0.850	0.846
60	0.400	0.401	0.600	0.601	0.850	0.851
70	0.400	0.404	0.600	0.605	0.850	0.856
80	0.400	0.403	0.600	0.604	0.850	0.855
90	0.400	0.401	0.600	0.601	0.850	0.852
100	0.400	0.396	0.600	0.595	0.850	0.846

The results of the numerical experiment show that when using undisturbed input data, the values of the desired function $\psi_e(t)$ are restored exactly (2,4, and 6th columns of Table 1). When using perturbed input data, in which the error has a fluctuating character, the values of the desired function are restored with a certain error (3,5 and 7th columns of Table 1). However, as follows from the table, the maximum relative error of restoring the values of the desired function $\psi_e(t)$ does not exceed 2.5%. When the error level decreases, the solution is restored more accurately. The analysis of the results of the numerical experiment shows that the proposed computational algorithm ensures the stability of the solution to input data errors.

To illustrate the possibility of practical application of the proposed method, numerical calculations were carried out for a hypothetical chemical reactor. As input parameters of the diffusion model of the hydrodynamic flow in the reactor, the following parameters were taken: $d = 0.38\,m^2/s$, $k = 0,2\,m^3/(kg \cdot s)$, $v(t) = 0,5\,m/s$, $\varphi(x) = 0$, $l = 3\,m$. It was necessary to determine the concentration of the selected reagent in the incoming stream$\psi_e(t)$, which provided a predetermined mode at the reactor outlet, $f(t) = 0.05; 0.1;$ 0.2; 0.3; 0.4; $0.5\,m^3/kg$. The results of numerical calculations carried out before entering the stationary mode of the process in the reactor are presented in Table 2.

Table 2. Results of numerical calculations for a hypothetical reactor

$f(t)$	0.05	0.1	0.2	0.3	0.4	0.5
$\psi_e(t)$	0.053	0.112	0.252	0.427	0.644	0.913

The analysis of the results of numerical experimentation indicates that the proposed computational algorithm makes it possible to determine the possibility of implementing a predetermined hydrodynamic regime at the reactor outlet.

5. Conclusion

The inverse problem related to the determination of the parameter in the flow entering the chemical reactor, which ensures the implementation of a predetermined hydrodynamic

regime at the reactor outlet, is considered. According to the proposed computational algorithm, the initial problem is first discretized, then the resulting difference problem is presented as a variational problem with local regularization, and a special representation is used to solve the variational problem. Unlike the global regularization method, where the solution of the inverse problem is determined for all time points simultaneously, the proposed approach takes into account the specifics of the inverse problem, and the solution is determined sequentially for individual time points.

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