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IDENTIFICATION OF THE COEFFICIENT IN THE DIFFUSION MODEL OF HYDRODYNAMIC FLOW IN A CHEMICAL REACTOR

A chemical technological process taking place in a chemical reactor with a second-order chemical reaction is considered. A one-parameter diffusion model for nonstationary flows is proposed for the mathematical description of the hydrodynamic flow in the reactor. Within the framework of the proposed model, the task is set to identify the longitudinal mixing coefficient according to an additionally specified condition regarding the concentration of the reagent under study at the outlet of the reactor.

A special representation is proposed for the diffusion terms in the hydrodynamic flow model in the reactor. The method of difference approximation is used to construct a discrete analogue of this model using explicit-implicit time approximation for diffusion terms. Decomposition is used to numerically solve the resulting system of linear difference equations, as a result of which the system of difference equations for each discrete value of a time variable splits into two mutually independent linear subsystems, each of which can be solved independently, independently of each other. As a result, an explicit formula was obtained for determining the approximate value of the longitudinal mixing coefficient in a hydrodynamic flow. Based on the proposed computational algorithm, numerical calculations were performed for model problems.

Keywords: diffusion model; longitudinal mixing coefficient; coefficient inverse problem; explicit-implicit approximation; difference problem.

Постановка проблеми. It is known that interconnected hydrodynamic, thermal and diffusion processes are carried out in chemical reactors, which create conditions for the chemical transformation of a substance. A large number of different types and designs of chemical reactors are used in chemical technology, which are classified according to a number of characteristics [1, 2]. The most common classification of chemical reactors is based on the hydrodynamic mode of motion of the reaction medium in reactors. Hydrodynamic models of ideal mixing; ideal displacement; diffusion models; cellular models; combined models are used to describe flows of different nature in chemical reactors [3 – 6]. For mathematical description, most of the real

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hydrodynamic flows in chemical reactors mainly use one-parameter and two-parameter diffusion models. 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. [6].

When modeling the processes occurring in chemical reactors, it is considered a very important step to provide the appropriate mathematical models with the necessary quantitative information, i.e. identification 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 controlling the chemical technological process using the constructed model largely depend. It should be noted that the parameters of all mathematical models of chemical and technological processes are mainly determined on the basis of experimental studies, which are associated with certain difficulties. In this regard, there is a need to identify the parameters of mathematical models of chemical and technological processes based on computational experiments. In this paper, to identify the longitudinal mixing coefficient, a numerical method is proposed based on solving the inverse problem for a one-parameter diffusion model of hydrodynamic flow in a chemical reactor during a second-order reaction.

Problem Statement and Solution Method.

Suppose that a chemical reactor, which is a tubular apparatus, continuously receives a reaction stream. The incoming stream moves only in one direction along the length of the reactor and at the same time a second-order chemical reaction takes place with the participation of the reagent under study in the stream. It is assumed that the change in the concentration of the reagent under study 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,

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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, in accordance with 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 course of a second-order chemical reaction

$$\frac{\partial\psi(x,t)}{\partial t}+v(t)\frac{\partial\psi(x,t)}{\partial x}+k\psi^2(x,t)=d\,\frac{\partial^2\psi(x,t)}{\partial x^2}\,,$$

$$0<x<l,\ \ 0<t\le T\,, \tag{1}$$

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

Suppose that at the initial moment of time $t=0$ 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

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

The boundary conditions at the inlet $x=0$ and outlet $x=l$ of the reactor are formulated on the basis of the Dankverts condition, according to which the sum of the flows of matter approaching the reactor boundary at the ends of the apparatus should be equal to the flow of matter departing from the boundary [4, 6]. As a result, we will have

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

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

where $\xi(t)$ is the concentration of the reagent under study in the incoming stream. Obviously, if you set the functions $v(t)$, $\xi(t)$, $\phi(x)$ and values of the constant parameters d, k, then by solving the problem (1) – (4), you can find the function $\psi(x,t)$, i.e. the distribution of the reagent concentration along the length of the reactor.

Now let's assume that along with the unknown function $\psi(x,t)$, the longitudinal mixing coefficient d is also unknown and identification of this parameter of the diffusion model is required. For this purpose, an additional condition is set regarding the concentration of the reagent under study at the outlet of the reactor

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

Thus, the task is to determine the function $\psi(x,t)$ and coefficient d satisfying equation (1) and conditions (2) – (5). The task (1) – (4) belongs to the class of coefficient inverse problems of mathematical physics [7 – 10]. It should be noted that the correctness of the formulation of coefficient inverse problems, the issues of the existence and uniqueness of their solution in various functional classes are studied in [10-14]. Numerical methods for solving problems of identifying coefficients for parabolic equations are considered in many papers [15 – 19].

Suppose that the coefficient inverse problem of determining the pair $(\psi(x,t),\ d)$ from equation (1) and conditions (2)–(5) is uniquely solvable.

Let's proceed to the construction of a discrete analog of the problem (1) – (5). To do this, we introduce a uniform space-time difference grid in a rectangular area $\{0 \le x \le l,\ \ 0 \le t \le T\}$

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

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where $\Delta x = \frac{l}{n}$ is the step of the difference grid in the variable x, $\Delta t = \frac{T}{m}$ is the step of the difference grid in time t. First, the diffusion terms $d\frac{\partial^2 \psi(x,t)}{\partial x^2}$ and $d\frac{\partial \psi(0,t)}{\partial x}$ in equation (1) and boundary condition (3) are represented as

$$d\frac{\partial^2 \psi(x,t)}{\partial x^2} = d_0\frac{\partial^2 \psi(x,t)}{\partial x^2} + d_1\frac{\partial^2 \psi(x,t)}{\partial x^2},$$

$$d\frac{\partial \psi(0,t)}{\partial x} = d_0\frac{\partial \psi(0,t)}{\partial x} + d_1\frac{\partial \psi(0,t)}{\partial x},$$

where $d = d_0 + d_1$, $d_0 > 0$ is a given value and d_1 is an unknown value.

Using the method of difference approximation, we construct a discrete analogue of the problem (1) – (5) on a grid $\bar{\omega}$, using an explicit– implicit time approximation for the above-presented diffusion terms

$$\frac{\psi_i^j - \psi_i^{j-1}}{\Delta t} + v^j\frac{\psi_i^j - \psi_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 = \\ = d_0\frac{\psi_{i+1}^j - 2\psi_i^j + \psi_{i-1}^j}{\Delta x^2} + d_1\frac{\psi_{i+1}^{j-1} - 2\psi_i^{j-1} + \psi_{i-1}^{j-1}}{\Delta x^2}, \quad (6)$$

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

$$v^j\xi^j + d_0\frac{\psi_1^j - \psi_0^j}{\Delta x} + d_1\frac{\psi_1^{j-1} - \psi_0^{j-1}}{\Delta x} = v^j\psi_0^j, \quad (7)$$

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

$$\psi_n^j = f^j, \quad (9)$$

$$j = 1, 2, \ldots, m,$$

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$$\psi_i^0 = \phi_i, \qquad i = 0,\ 2,\ \ldots n, \tag{10}$$

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

As can be seen, the discrete analogue of the problem (1) – (5) for each fixed value j, $j = 1, .2 \ldots, m$ is a system of linear algebraic equations in which the magnitude d_1 and approximate values of the desired function $\psi(x,t)$ in the nodes of the difference grid $\overline{\omega}$ act as unknowns , i.e. ψ_i^j, $i = 0, 1, 2, \ldots, n-1$, $j = 1, 2, 3, \ldots., m$.

To solve the resulting system of difference equations (6) – (10), we use the idea of decomposing this system into mutually independent subsystems, each of which can be solved independently, independently of each other [9, 17]. For this purpose, the solution of the system of equations (6) – (10) for each fixed value $j = 1, 2, \ldots., m$ is represented as

$$\psi_i^j = u_i^j + d_1 w_i^j, \qquad i = 0, 1, 2, \ldots, n, \tag{11}$$

where u_i^j, w_i^j are also unknown variables. Substituting the ratio (11) into equation (6), we will have

$$\frac{u_i^j + d_1 w_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{u_i^j + d_1 w_i^j - u_{i-1}^j - d_1 w_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 =$$

$$= d_0 \frac{u_{i+1}^j + d_1 w_{i+1}^j - 2u_i^j - 2d_1 w_i^j + u_{i-1}^j + d_1 w_{i-1}^j}{\Delta x^2} +$$

$$+ d_1 \frac{\psi_{i+1}^{j-1} - 2\psi_i^{j-1} + \psi_{i-1}^{j-1}}{\Delta x^2}$$

or

$$\left[\frac{u_i^j - \psi_i^{j-1}}{\Delta t} + v^j \frac{u_i^j - u_{i-1}^j}{\Delta x} + k(\psi_i^{j-1})^2 - d_0 \frac{u_{i+1}^j - 2u_i^j - u_{i-1}^j}{\Delta x^2}\right] +$$

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$$+d_1\left[\frac{w_i^j}{\Delta t}+v^j\frac{w_i^j-w_{i-1}^j}{\Delta x}-d_0\frac{w_{i+1}^j-2w_i^j+w_{i-1}^j}{\Delta x^2}-\frac{\psi_{i+1}^{j-1}-2\psi_i^{j-1}+\psi_{i-1}^{j-1}}{\Delta x^2}\right]=0\,.(12)$$

And the substitution expression ψ_i^j in (7), (8)

$$\left[v^j\xi^j+d_0\frac{u_1^j-u_0^j}{\Delta x}-v^ju_0^j\right]+d_1\left[d_0\frac{w_1^j-w_0^j}{\Delta x}+\frac{\psi_1^{j-1}-\psi_0^{j-1}}{\Delta x}-v^jw_0^j\right]=0\,,(13)$$

$$\frac{u_n^j-u_{n-1}^j}{\Delta x}+d_1\frac{w_n^j-w_{n-1}^j}{\Delta x}=0\,. \qquad (14)$$

Obviously, the relations (12) – (14) will be executed automatically for each fixed value j, $j=1, 2, \ldots, m$, if:

the variables u_i^j, $i=0,1,2,..,n$ satisfy the system of difference equations

$$\frac{u_i^j-\psi_i^{j-1}}{\Delta t}+v^j\frac{u_i^j-u_{i-1}^j}{\Delta x}+k(\psi_i^{j-1})^2-d_0\frac{u_{i+1}^j-2u_i^j-u_{i-1}^j}{\Delta x^2}=0\,, \qquad (15)$$

$$v^j\xi^j+d_0\frac{u_1^j-u_0^j}{\Delta x}-v^ju_0^j=0\,, \qquad (16)$$

$$\frac{u_n^j-u_{n-1}^j}{\Delta x}=0\,, \qquad (17)$$

and the variables w_i^j, $i=0,1,2,..,n$ satisfy the following system of difference

$$\frac{w_i^j}{\Delta t}+v^j\frac{w_i^j-w_{i-1}^j}{\Delta x}-d_0\frac{w_{i+1}^j-2w_i^j+w_{i-1}^j}{\Delta x^2}-\frac{\psi_{i+1}^{j-1}-2\psi_i^{j-1}+\psi_{i-1}^{j-1}}{\Delta x^2}=0\,,(18)$$

$$d_0\frac{w_1^j-w_0^j}{\Delta x}+\frac{\psi_1^{j-1}-\psi_0^{j-1}}{\Delta x}-v^jw_0^j=0\,, \qquad (19)$$

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$$\frac{w_n^j - w_{n-1}^j}{\Delta x} = 0. \qquad (20)$$

The obtained independent systems of difference equations (15) – (17) and (18)–(20) for each fixed value j, $j = 1, 2, \ldots, m$ are a system of linear algebraic equations with a tridiagonal matrix, the solutions of which are determined by the well-known Thomas method [9].

Substituting representation (11) into (9), we will have

$$u_n^j + d_1 w_n^j = f^j.$$

From here we get a formula for determining the approximate value of an unknown quantity d_1

$$d_1 = \frac{f^j - u_n^j}{w_n^j}.$$

And to calculate the approximate value of the desired longitudinal mixing coefficient d, we will have

$$d = d_0 + d_1 = d_0 + \frac{f^j - u_n^j}{w_n^j}. \qquad (21)$$

Thus, the computational algorithm for solving the system of difference equations (6)–(10) by definition ψ_i^j, $i = 0, 1, 2, .., n$, and d, at each time layer j, $j = 1, 2, ..., m$, consists of the following stages:

1) the solutions of two independent systems of difference equations (15) – (17) and (18) – (20) with respect to auxiliary variables are determined u_i^j, w_i^j, $i = 0, 1, 2, .., n$;

2) The approximate value of the desired longitudinal mixing coefficient d is determined by the formula (21) ;

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3) The values of the variables ψ_i^j, $i = 0, 1, 2, .., n$ are calculated using the formula (11).

In order to test the effectiveness of the proposed computational algorithm, numerical experiments were conducted for model problems. The numerical experiments were carried out according to the following scheme:

I. For a given value of the longitudinal mixing coefficient d, the solution of the direct problem (1) – (4), i.e. the function $\psi(r,t)$, $0 \le x \le l$, $0 \le t \le T$, is determined ;

II. The dependence $f(t) = \psi(l,t)$ is taken as the exact input data for solving the inverse problem of d recovery.

The results of numerical experiments show that the proposed computational algorithm can be applied in the study of hydrodynamic flows in chemical reactors.

Conclusion.

The problem of identification of the longitudinal mixing coefficient in a one-parameter diffusion model of hydrodynamic flow in a chemical reactor is considered. When constructing a discrete analogue of the nonlinear problem under consideration, an explicit-implicit approximation in time is used for the diffusion terms. This makes it possible to reduce a nonlinear problem to solving a system of linear difference equations. And the proposed decomposition of the resulting system allows us to find the coefficient of longitudinal mixing using an explicit formula. The proposed method can also be used to identify the parameters of a two-parameter diffusion model of a hydrodynamic flow.

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Ідентифікація коефіцієнта дифузійної моделі гідродинамічного потоку в хімічному реакторі / Ханлар Мехвали оглу Гамзаєв, Нушаба Ханлар гизи Байрамова // Вісник НТУ "ХПІ". Серія: Інформатика та моделювання. – Харків: НТУ "ХПІ". – 2024. – № 1 – 2 (11 – 12). – С. 15 – 26.

Розглядається хіміко-технологічний процес, що протікає у хімічному реакторі, з хімічною реакцією другого порядку. Для математичного опису гідродинамічного потоку в реакторі пропонується однопараметрична дифузійна модель нестаціонарних потоків. В рамках запропонованої моделі поставлено завдання ідентифікації коефіцієнта поздовжнього перемішування додатково заданою умовою щодо концентрації досліджуваного реагенту на виході з реактора.

Пропонується спеціальне подання для дифузійних членів моделі гідродинамічного потоку в реакторі. Методом різницевої апроксимації будується дискретний аналог даної моделі з використанням явно-неявної апроксимації за часом для дифузійних членів. Для чисельного рішення отриманої системи лінійних різницевих рівнянь застосовується декомпозиція, у результаті система різницевих рівнянь при кожному дискретному значенні тимчасової змінної розпадається дві взаємно незалежні лінійні підсистеми, кожна з яких може вирішуватися самостійно, незалежно друг від друга. В результаті отримана явна формула для визначення наближеного значення коефіцієнта поздовжнього перемішування гідродинамічному потоці. На основі запропонованого обчислювального алгоритму було проведено чисельні розрахунки для модельних завдань. Бібліогр.: 19 назв.

Ключові слова*:* дифузійна модель; коефіцієнт поздовжнього перемішування; коефіцієнтне зворотне завдання; явно-неявна апроксимація; різницеве завдання.

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This article analyzes in detail the actual problem of the spread of disinformation through various media resources and their impact on society. The main aspects of information consumption by Ukrainian society, in particular on the Internet, are highlighted, and the potential target audience is determined. Based on the analysis, a new intelligent system based on Natural Language Processing technology is proposed, which provides users with a comprehensive overview of the activity of each media resource. Available analogues with their advantages and limitations are examined in detail, emphasizing the significant advantages of the proposed intelligent system for increasing information literacy and countering disinformation. Refs.: 19 titles.

Keywords: diffusion model; longitudinal mixing coefficient; coefficient inverse problem; explicit-implicit approximation; difference problem.