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IDENTIFICATION OF THE BOUNDARY CONDITION IN THE DIFFUSION MODEL OF THE HYDRODYNAMIC FLOW IN A CHEMICAL REACTOR

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The motion of a hydrodynamic flow in a chemical reactor described by a one-dimensional one-parameter diffusion model is considered. Within the framework of this model, the task is set to identify the boundary condition at the reactor outlet containing an unknown concentration of the reagent under study leaving the reactor in a stream. In this case, the law of change in the concentration of the reagent over time at the reactor inlet is additionally set. After the introduction of dimensionless variables, a discrete analogue of the transformed inverse problem in the form of a system of linear algebraic equations is constructed by the method of difference approximation. The discrete analogue of the additional condition is written as a functional and the solution of a system of linear algebraic equations is presented as a variational problem with local regularization. A special representation is proposed for the numerical solution of the constructed variational problem. As a result, the system of linear equations for each discrete value of a dimensionless time splits into two independent linear subsystems, each of which is solved independently of each other. As a result of minimizing the functional, an explicit formula was obtained for determining the approximate concentration of the reagent under study in the flow leaving the reactor at each discrete value of the dimensionless time. The proposed computational algorithm has been tested on the data of a model chemical reactor.

Keywords: chemical reactor; one-parameter diffusion model; Peclet parameter; boundary inverse problem; local regularization method.

Introduction

It is known that a chemical reactor in which interconnected hydrodynamic, thermal, and diffusion processes are carried out [1–3] is a central element in any chemical technology system. To describe various hydrodynamic flows in chemical reactors, models are used: ideal mixing; ideal displacement; diffusion models; cellular models; and combined models [4–7]. For mathematical description, most of the real 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. 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. [1, 3].

Usually, when studying the processes occurring in a chemical reactor based on a diffusion model, the geometric parameters of the reactor, the initial state of the reactor, as well as the conditions at the inlet and outlet of the reactor are considered set. However, it

is necessary to note a very important circumstance regarding the conditions set at the exit from the reactor. The fact is that the regime at the reactor outlet is established during two interacting processes in the reactor – convective transport and diffusion (convective diffusion). For this reason, the output mode of the reactor cannot be adjusted according to a predetermined program. Therefore, it is practically impossible to accurately represent the conditions at the reactor outlet. In this regard, for the processes of chemical technology, the task of identifying the boundary condition at the reactor outlet is important only based on the specified information at the reactor entrance.

1. Problem Statement and Solution Method

Suppose that a hydrodynamic flow continuously enters a chemical reactor, which is a tubular apparatus, and the incoming flow moves only in one direction along the length of the reactor. It is assumed that the reactor operates in an isothermal mode and a change in the concentration of the reagent (understudy) in the reactor occurs due to its transfer by hydrodynamic flow (convective transfer) and because of its transfer by diffusion (diffusion transfer). In the reactor, only longitudinal mixing of the reagent takes place in the flow and the values of the flow parameters along the reactor section are the same. To mathematically describe the motion of the hydrodynamic flow in this chemical reactor, we use a one-dimensional, one-parameter diffusion flow model [5, 6]

$$\frac{\partial C(x,t)}{\partial t} + u\frac{\partial C(x,t)}{\partial x} = d\frac{\partial^2 C(x,t)}{\partial x^2}, \quad 0 < x < l,\ 0 < t \le t_0, \tag{1}$$

where $C(x,t)$ is the concentration of the reagent, u is the rate of hydrodynamic flow in the reactor, d is the coefficient of turbulent diffusion, l is the length of the chemical reactor, x is the coordinate along which the hydrodynamic flow moves, t is a time.

Suppose 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

$$C(x,0) = \psi(x), \quad 0 \le x \le l. \tag{2}$$

The boundary conditions at the inlet $x = 0$ and outlet $x = l$ of the reactor are formulated according to the Danckwerts condition [5, 8]: the sum of the flows of matter approaching the reactor boundary should be equal to the flow of matter departing from the boundary. As a result, we will have

$$u\xi(t) + d\frac{\partial C(0,t)}{\partial x} = uC(0,t), \tag{3}$$

$$u\theta(t) + d\frac{\partial C(l,t)}{\partial x} = uC(l,t), \tag{4}$$

where $\xi(t)$ is the concentration of the reagent in the stream entering the reactor, $\theta(t)$ is the concentration of the reagent in the stream leaving the reactor. If you set the functions $\psi(x)$, $\xi(t)$, $\theta(t)$ and values of the constant parameters u and d, then solve the problem (1) – (4), you can find the function $C(x,t)$, i.e., the distribution of the reagent concentration along the length of the reactor. However, the concentration of the reagent in the flow leaving the reactor $\theta(t)$ is set during the processes in the reactor and it is not

possible to regulate it according to a given program. Therefore, the function $\theta(t)$ is also unknown and must be defined along with the function $C(x,t)$. Obviously, in this case, an additional condition must be set for the correct formulation of the problem. Suppose that at the reactor inlet $x=0$, the law of change in the concentration of the reagent over time is set. Then we will have an additional condition on this boundary

$$C(0,t)=f(t). \tag{5}$$

Thus, the task is to determine the functions $C(x,t)$ and $\theta(t)$ satisfying equation (1) and conditions (2) – (5). It should be noted that due to the incorrectness of the boundary condition (5) for equation (1), problem (1) – (5) is considered incorrectly posed and belongs to the class of boundary inverse problems [9–12]. The issues of the correctness of the statements of boundary inverse problems, the issues of the existence and uniqueness of their solutions in various functional classes are studied in [9, 10, 13–15]. Numerous papers have been devoted to the development of numerical methods for solving inverse problems related to the identification of boundary conditions [9, 11, 16–19].

Let's introduce dimensionless variables

$$y=\frac{x}{l},\quad \tau=\frac{t}{l/u}$$

and the problem (1) – (5) is represented as

$$\frac{\partial C(y,\tau)}{\partial \tau}+\frac{\partial C(y,\tau)}{\partial y}=\frac{1}{Pe}\frac{\partial^2 C(y,\tau)}{\partial y^2},\quad 0<y<1,\ \ 0<\tau\le T, \tag{6}$$

$$C(y,0)=\psi(y),\quad 0\le y\le 1, \tag{7}$$

$$\xi(\tau)+\frac{1}{Pe}\frac{\partial C(0,\tau)}{\partial y}=C(0,\tau), \tag{8}$$

$$\theta(\tau)+\frac{1}{Pe}\frac{\partial C(1,\tau)}{\partial \tau}=C(1,\tau), \tag{9}$$

$$C(0,\tau)=f(\tau), \tag{10}$$

where $T=\dfrac{t_0}{l/u}$, $Pe=\dfrac{lu}{d}$ are a dimensionless Peclet parameter.

Using the method of difference approximation, we construct a discrete analogue of the boundary inverse problem (6) – (10), assuming that there is a solution to this problem and it is the only one. To this end, we discretize a given rectangular area $\{0\le y\le 1,\ \ 0\le\tau\le T\}$ in space and in time, with steps $\Delta y=1/n$ by variable y and $\Delta\tau=T/m$ by variable τ

$$\overline{\omega}=\{(y_i,\tau_j):\ y_i=i\Delta y,\ \ \tau_j=j\Delta\tau,\ \ i=0,\,1,\,2,...,n,\ \ j=0,\,1,\,2,\ldots,m\}.$$

The discrete analogue of the problem (6) – (10) on the difference grid $\overline{\omega}$ is represented as

$$\frac{C_i^j-C_i^{j-1}}{\Delta\tau}+\frac{C_i^j-C_{i-1}^j}{\Delta y}=\frac{1}{Pe}\frac{C_{i+1}^j-2C_i^j+C_{i-1}^j}{\Delta y^2},\ i=1,\ 2,\ldots,n-1, \tag{11}$$

$$\xi^j + \frac{1}{Pe}\frac{C_1^j - C_0^j}{\Delta y} = C_0^j, \tag{12}$$

$$\theta^j + \frac{1}{Pe}\frac{C_n^j - C_{n-1}^j}{\Delta y} = C_n^j, \tag{13}$$

$$C_0^j = f^j, j = 1, 2, \ldots, m, \tag{14}$$

$$C_i^0 = \psi_i, \quad i = 0,\ 2, \ldots, n, \tag{15}$$

where $C_i^j \approx C(y_i, \tau_j)$, $\psi_i = \psi(y_i)$, $f^j = f(\tau_j)$, $\xi^j \approx \xi(\tau_j)$, $\theta^j = \theta(\tau_j)$.

The linear system of difference equations (11) – (15) for each fixed value j, $j = 1, 2, \ldots, m$ is represented as a variational problem with local regularization [11]. To do this, in accordance with (14), we introduce a smoothing functional in the form

$$J(\theta^j) = \left[C_0^j - f^j\right]^2 + \alpha(\theta^j)^2 \to \min, \tag{16}$$

where α is a regularization parameter. Thus, the task of determining the concentration of the reagent in the flow leaving the reactor θ^j at each fixed value $j = 1, 2, \ldots, m$ is reduced to the task of minimizing the smoothing functional (16) when conditions (11) – (13) are met. To decompose the system of difference equations (11) – (13) into mutually independent subsystems, its solution for each fixed value $j = 1, 2, \ldots, m$ is represented as [11, 16]

$$C_i^j = V_i^j + \theta^j W_i^j, \quad i = 0,\ 1,\ 2,\ \ldots,\ n, \tag{17}$$

where V_i^j, W_i^j and θ^j are a unknown variables.

Substituting the ratio (17) into equation (11), we will have:

$$\frac{V_i^j + \theta^j W_i^j - C_i^{j-1}}{\Delta\tau} + \frac{V_i^j + \theta^j W_i^j - V_{i-1}^j - \theta^j W_{i-1}^j}{\Delta y} =$$

$$= \frac{1}{Pe}\frac{V_{i+1}^j + \theta^j W_{i+1}^j - 2V_i^j - 2\theta^j W_i^j + V_{i-1}^j + \theta^j W_{i-1}^j}{\Delta y^2}$$

or

$$\left[\frac{V_i^j - C_i^{j-1}}{\Delta\tau} + \frac{V_i^j - V_{i-1}^j}{\Delta y} - \frac{1}{Pe}\frac{V_{i+1}^j - 2V_i^j + V_{i-1}^j}{\Delta y^2}\right] +$$

$$+ \theta^j\left[\frac{W_i^j}{\Delta\tau} + \frac{W_i^j - W_{i-1}^j}{\Delta y} - \frac{1}{Pe}\frac{W_{i+1}^j - 2W_i^j + W_{i-1}^j}{\Delta y^2}\right] = 0.$$

Substituting the representation (17) into (12), (13), gives

$$\left[\frac{1}{Pe}\frac{V_1^j - V_0^j}{\Delta y} - V_0^j + \xi^j\right] + \theta^j\left[\frac{1}{Pe}\frac{W_1^j - W_0^j}{\Delta y} - W_0^j\right] = 0,$$

$$\left[\frac{1}{Pe}\frac{V_n^j - V_{n-1}^j}{\Delta y} - V_n^j\right] + \theta^j\left[\frac{1}{Pe}\frac{W_n^j - W_{n-1}^j}{\Delta y} - W_n^j + 1\right] = 0.$$

Suppose that the auxiliary variables V_i^j and W_i^j are solutions of the following two independent systems of difference equations

$$\frac{V_i^j - C_i^{j-1}}{\Delta\tau} + \frac{V_i^j - V_{i-1}^j}{\Delta y} - \frac{1}{Pe}\frac{V_{i+1}^j - 2V_i^j + V_{i-1}^j}{\Delta y^2} = 0, \tag{18}$$

$$\frac{1}{Pe}\frac{V_1^j - V_0^j}{\Delta y} - V_0^j + \xi^j = 0, \tag{19}$$

$$\frac{1}{Pe}\frac{V_n^j - V_{n-1}^j}{\Delta y} - V_n^j = 0, \tag{20}$$

$$\frac{W_i^j}{\Delta\tau} + \frac{W_i^j - W_{i-1}^j}{\Delta y} - \frac{1}{Pe}\frac{W_{i+1}^j - 2W_i^j + W_{i-1}^j}{\Delta y^2} = 0, \tag{21}$$

$$\frac{1}{Pe}\frac{W_1^j - W_0^j}{\Delta y} - W_0^j = 0, \tag{22}$$

$$\frac{1}{Pe}\frac{W_n^j - W_{n-1}^j}{\Delta y} - W_n^j + 1 = 0. \tag{23}$$

Obviously, when using decomposition (17), equation (11) and conditions (12), (13) are fulfilled automatically at any θ^j.

The systems of difference equations (18) – (20) and (21) – (23) for each fixed value j, $j = 1, 2, \ldots, m$ are a system of linear algebraic equations with a tridiagonal matrix and solutions of these systems can be found by the Thomas method [11]. Substituting representation (17) into (16), we will have

$$J(\theta^j) = \left[V_0^j + \theta^j W_0^j - f^j\right]^2 + \alpha(\theta^j)^2 \to \min.$$

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

$$\left[V_0^j + \theta^j W_0^j - f^j\right] W_0^j + \alpha\theta^j = 0.$$

From here we obtain a formula for determining the approximate value of the desired function $\theta(\tau)$at $\tau = \tau_j$, i.e. θ^j

$$\theta^j = \frac{W_0^j(f^j - V_0^j)}{(W_0^j)^2 + \alpha}. \tag{24}$$

Thus, a computational algorithm for solving a variational problem with local regularization (11) – (13), (16) by definition C_i^j and θ^j, $i = 0, 1, 2, \ldots, n$, for each fixed value j, $j = 1, 2, \ldots, m$, consists of the following stages:

I. In parallel, solutions of two independent systems of difference equations (18) – (20) and (21) – (23) concerning auxiliary variables V_i^j, W_i^j, $i = 0, 1, 2, \ldots, n$.

II. According to formula (24), the approximate value of the desired function $\theta(\tau)$ is determined at $\tau = \tau_j$, i.e. θ^j.

III. The values of the variables C_i^j, $i = 0, 1, 2, \ldots, n$ are calculated using the formula (17).

2. The Results of Numerical Calculations

The proposed computational algorithm has been tested on the data of a model reactor. The numerical experiment was carried out in the following sequence:

1) the functions $\psi(y)$, $\xi(\tau)$, $\theta(\tau)$ and the parameter value Pe are set . The solution of the problem (6) – (9) is determined, i.e. the function $C(y,\tau)$, $0 \le y \le 1$, $0 \le \tau \le T$;

2) the found dependence $f(\tau) = C(0,\tau)$ is taken as the exact input data for solving the inverse problem of recovery $\theta(\tau)$.

Both undisturbed and perturbed input data were used in numerical calculations to restore $\theta(\tau)$. When using undisturbed input data, the value of the regularization parameter α is assumed to be zero. In order to perturb the input data, a random variable $\sigma(\tau)$ is used, modeled using a random number sensor, and the perturbed data is determined by the formula

$$\tilde{f}(\tau) = f(\tau) + \delta\sigma(\tau)f(\tau)\,,$$

δ is the level of error. The term $\delta\sigma(\tau)f(\tau)$ simulates a different level of error for the input data $f(\tau)$. In this case, the value of the regularization parameter α is determined in accordance with the principle of discrepancy [9, 11].

Numerical experiments were carried out on a uniform difference grid with steps $\Delta\tau = 0,5$, $\Delta y = 5\cdot 10^{-3}$, for the following functions $\theta(\tau) = 0,2+0,1\sin 10\tau$; $\theta(\tau) = 1-0,2e^{-0,2\tau}$ kg/m^3 at $\xi(\tau)$= 0,5 kg/m^3, $\psi(y) = 0$, $Pe = 0,5$ and $Pe = 5$. To perturb the input data, the following was used as the error level $\delta = 2\cdot 10^{-4}$.

The results of numerical experiments conducted with undisturbed and perturbed input data are presented in Table 1; in it τ– the dimensionless time,θ^e it contains the exact values of the desired function $\theta(\tau)$, $\bar{\theta}$ and $\tilde{\theta}$– the calculated values $\theta(\tau)$ with undisturbed and perturbed input data. Table 1 also shows the dimensionless time change in the concentration of the reagent at the reactor inlet f^j.

The results of numerical experiments show that when using undisturbed input data, the values of the desired function $\theta(\tau)$ are restored exactly (the second, third and sixth, seventh columns of the table 1). When using perturbed input data, in which the error has a fluctuating character, the values of the desired function are restored with an error (fourth and eighth columns of the table). However, it follows from the table 1 that at a given level of error, the maximum relative error in restoring the values of the desired function $\theta(t)$ does not exceed 2,41% and 2,32%, respectively. At the same time, the value of the local regularization parameter assumed the value $\alpha = 5\cdot 10^{-4}$and $\alpha = 10^{-6}$, respectively.

To illustrate the possibility of practical application of the proposed method, numerical calculations were performed for a hypothetical chemical reactor. As input parameters of the diffusion model of the hydrodynamic flow in the reactor, the following parameters were set: $\xi(t)$ is a concentration of the reagent in the stream entering the reactor, $f(t)$ is a reagent concentration at the reactor inlet $x = 0$, Pe is a Peclet parameter and $\psi(x) = 0$ is a distribution of the reagent concentration along the length of the reactor at the initial time. It is required to determine the concentration of the reagent in the flow leaving the reactor $\theta(t)$. The results of numerical calculations carried out before entering the stationary mode of the process in the reactor are presented in Table 2.

The analysis of the results of numerical experimentation indicates that the proposed computational algorithm can be used to determine the conditions in the reactor under which a predetermined hydrodynamic regime at the reactor outlet can be implemented.

Table 1

The results of numerical experiments to determine $\theta(\tau)$

τ	$\theta(\tau) = 0,2 + 0,1 \sin 10\tau$ $Pe = 0,5$			f^j	$\theta(\tau) = 1 - 0,2 \cdot e^{-0,2\tau}$ $Pe = 5$			f^j
	θ^e	θ	θ		θ^e	θ	θ	
1	0,146	0,146	0,145	0,382	0,836	0,836	0,851	0,441
2	0,291	0,291	0,291	0,564	0,866	0,866	0,885	0,454
3	0,101	0,101	0,101	0,831	0,890	0,890	0,889	0,436
4	0,275	0,275	0,274	1,063	0,910	0,910	0,907	0,412
5	0,174	0,174	0,174	1,271	0,926	0,926	0,929	0,382
6	0,170	0,170	0,169	1,556	0,940	0,940	0,933	0,347
7	0,277	0,277	0,277	1,738	0,951	0,951	0,940	0,307
8	0,101	0,101	0,100	2,019	0,960	0,960	0,950	0,260
9	0,289	0,289	0,290	2,240	0,967	0,967	0,974	0,207
10	0,149	0,149	0,151	2,465	0,973	0,973	0,979	0,145
11	0,196	0,196	0,195	2,746	0,978	0,978	0,980	0,075
12	0,258	0,258	0,259	2,933	0,982	0,982	0,982	0,006
13	0,107	0,107	0,107	3,225	0,985	0,985	0,986	0,098
14	0,298	0,298	0,298	3,437	0,988	0,988	0,987	0,204
15	0,129	0,129	0,130	3,680	0,990	0,990	0,982	0,325
16	0,222	0,222	0,222	3,954	0,992	0,992	0,985	0,463
17	0,235	0,235	0,237	4,149	0,993	0,993	0,974	0,621
18	0,120	0,120	0,119	4,449	0,995	0,995	0,989	0,801
19	0,300	0,300	0,298	4,654	0,996	0,996	1,019	1,008
20	0,113	0,113	0,115	4,915	0,996	0,996	0,974	1,243

Table 2

Results of numerical calculations for a hypothetical reactor

$\xi^j, \quad f^j$	θ^j		
	$Pe = 0,5$	$Pe = 2,0$	$Pe = 5,0$
0,5; 0,6	0,500	0,507	0,840
1,0; 1,2	1,001	1,014	1,681
1,5; 1,6	1,500	1,507	1,840

Conclusion

The problem of identifying a function included in the boundary condition and describing the concentration of the reagent under study in the flow leaving the reactor is considered. After the introduction of dimensionless variables, the problem is discretized and the resulting system of difference equations is presented as a variational problem with local regularization, for which a special representation is proposed.

The proposed computational algorithm allows, according to a predetermined hydrodynamic regime at the reactor entrance, to calculate the parameters of the hydrodynamic flow at the reactor outlet.

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ИДЕНТИФИКАЦИЯ ГРАНИЧНОГО УСЛОВИЯ В ДИФФУЗИОННОЙ МОДЕЛИ ГИДРОДИНАМИЧЕСКОГО ПОТОКА В ХИМИЧЕСКОМ РЕАКТОРЕ

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Рассматривается движение гидродинамического потока в химическом реакторе, описываемое одномерной однопараметрической диффузионной моделью. В рамках данной модели поставлена задача идентификации граничного условия на выходе реактора, содержащего неизвестную концентрацию исследуемого реагента, выходящего из реактора потоке. При этом дополнительно задается закон изменения концентрации реагента во времени на входе реактора. После введения безразмерных переменных, методом разностной аппроксимации построен дискретный аналог преобразованной обратной задачи в виде системы линейных алгебраических уравнений. Дискретный аналог дополнительного условия записывается в виде функционала и решение системы линейных алгебраических уравнений представляется как вариационная задача с локальной регуляризацией. Для численного решения построенной вариационной задачи предлагается специальное представление. В результате система линейных уравнений при каждом дискретном значении безразмерной времени распадается на две независимые линейные подсистемы, каждая из которых решается независимо друг от друга. В результате минимизации функционала получена явная формула для определения приближенного значения концентрации исследуемого реагента в потоке, выходящего из реактора, при каждом дискретном значении безразмерной времени. Предложенный вычислительный алгоритм опробован на данных модельного химического реактора.

Ключевые слова: химический реактор; однопараметрическая диффузионная модель; параметр Пекле; граничная обратная задача; метод локальной регуляризации.

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