

Software system for identifying diffusion parameters in microporous samples^{*}

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Abstract

An approach is proposed to implement a software system designed to identify diffusion parameters in samples of zeolite materials. For this purpose, mathematical models of direct and inverse diffusion problems are constructed, and their equivalent finite-difference schemes are obtained. For the mathematical model of the inverse diffusion problem, a software module is developed that works with experimental data, transforming them into a format suitable for applying an algorithmic difference scheme to determine diffusion coefficients. For the mathematical model of the direct diffusion problem, a software module is built that implements mass transfer processes in samples with cylindrical geometry. The developed architecture of the software system allows users to efficiently and clearly work with its components and, according to needs, change the physicochemical and geometric parameters of samples. Verification of the software system's operation is performed by testing the joint operation of its components and comparing experimental data from the inverse problems with the results obtained from the direct mathematical model.

Keywords

inverse problem, mathematical model, identification of diffusion parameters

1. Introduction

Processing a significant amount of data obtained during experimental studies in most exact and natural sciences, as well as during the monitoring of technological processes, almost always leads to the need to establish a general set of active parameters that act as factors determining the spatial and temporal dependencies of the studied processes. Such problems have long gone beyond the boundaries of classical disciplines and fields; for effective work, it is necessary to apply and develop new methods that belong to the subject areas of software engineering and computer science.

The mentioned problems have been increasingly arising in recent years in the study of diffusion transfer processes in various functional materials – zeolites, which have a complex microporous structure [1-3]. Working with data obtained from research on such materials requires specialized software, which often needs to be developed separately for each type of material and which is characterized by weak variability in manipulating input parameters [4, 5].

It becomes obvious that to approach the solution of the problem of developing such software, it is necessary to break it down into component subsystems, and to divide the process itself into several steps. In the general case, the necessary parameters can be established in several stages. At the first stage, mathematical models of the processes should be constructed, and by substituting experimentally obtained data, the inverse problem should be solved, which will allow identifying the necessary parameters, in particular, diffusion coefficients. At the second stage, the obtained parameters should be used to verify more general models, changing the input parameters of

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materials, their precision characteristics. The final stage is the development of the software system architecture, an interface that ensures user interaction with the software system, which will allow its specification and, to a certain extent, ensure its general nature. In the proposed paper, the mentioned problems are solved by developing mathematical models for the direct and inverse diffusion problems in microporous functional materials with cylindrical geometry. For the developed mathematical models, their representation in the form of finite-difference schemes approximating the original mass transfer equations, initial and boundary conditions to them is performed. The architecture of a software system is developed, which consists in distributed work with its components, changing the input parameters of samples, the ability to process input data necessary for working with parameter identification problems. The possibility of direct use of identified diffusion parameters in direct mathematical modeling of hydrocarbon mass transfer for various samples is provided, as well as the possibility of further complication of these models and the functionality of the software system itself.

2. Development of direct and inverse problems for a mathematical diffusion model in microporous materials. Designing the architecture of a software system implementing the mathematical model

2.1. Problem statement. Obtaining and processing experimental data on diffusion processes in studied samples

Experimental data related to mass transfer in zeolite samples at different temperature regimes usually concerns the diffusion of gas mixtures [6-10], often mixtures of volatile hydrocarbons: methane and propane, or benzene and hexane, taken in various proportions. The main problem of such studies is that it is experimentally or technologically impossible to establish the real ratio between the components of the working agent and impurities.

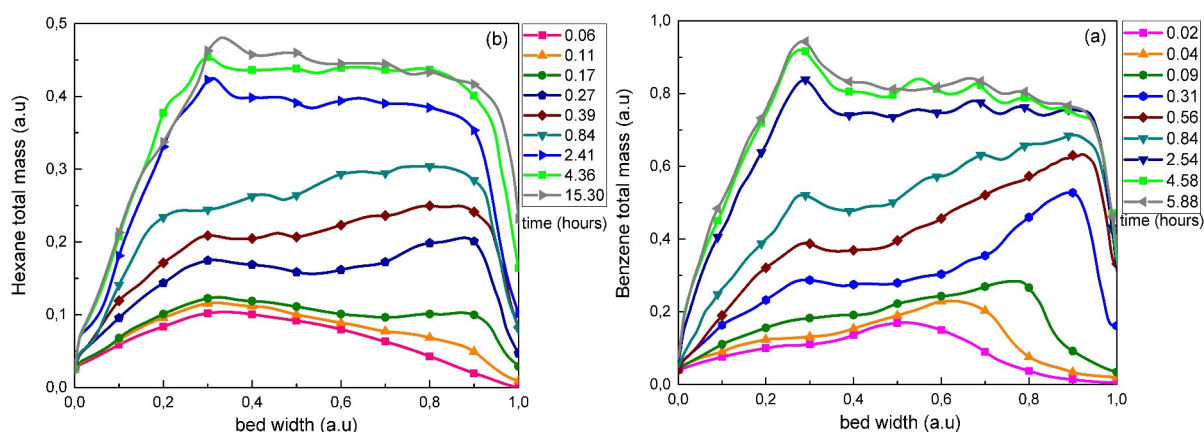


Figure 1: Examples of experimental absorption curves of a hydrocarbon mixture with a predominance of benzene (a) and hexane (b) in different time regimes (in hours).

Figure 1a, b shows typical dependencies of concentration distributions for the diffusion of benzene and hexane, respectively, at different time points depending on the geometric dimensions of the studied zeolite sample. These experimental data represent the results that a mathematical model could give us for the direct diffusion problem. Now, with known concentrations, by substituting the experimental data into the system of diffusion equations, it is possible to solve the problem of determining its main parameters.

The main problem of mathematical modeling in this case is the determination of diffusion parameters in the studied systems at different time points. These characteristics are the diffusion

coefficients in the micropore environment and the crystalline sample environment. Determining these parameters from experimental data would solve the problem of identifying the diffusion of mixtures and reliably predict the kinetics of mass transfer in the studied samples. The posed problem actually reduces to the identification of diffusion coefficients from the inverse problem for a mathematical model with feedback. In fact, our ultimate goal is to develop a software system that, firstly, implements the inverse problem for the mathematical model of diffusion and, secondly, allows, without delving into the physicochemical essence of the process, to determine the diffusion coefficients from the concentration distribution and effectively predict what substance we are dealing with. Development of a mathematical model of an inverse mathematical model and a software system that implements this model and its architecture is discussed further.

2.2. Mathematical model of diffusion in microporous materials. Description of the diffusion process within micropores and the bulk environment of a crystalline sample

To describe the diffusion process in a microporous material, an adequate mathematical model should be constructed that describes mass transfer in a wide time regime and in all subsystems of the studied sample. As is known [10-12], diffusion in microporous materials occurs simultaneously within two subsystems. The first subsystem characterizes diffusion in the general environment of the crystalline continuum; we will assume that this environment is characterized by the diffusion coefficient D_{inter} . The second subsystem describes the important process of capturing the working agent by micropores, i.e., the mass transfer process inside the pore itself. We will consider that this environment is characterized by the diffusion coefficient D_{intra} .

We will assume that the studied sample is characterized by cylindrical symmetry and has a characteristic length l . We will also assume that the micropores contained within the sample have the same size and a spherical shape with radius R . An example of such a zeolite sample along with micropores is shown in Figure 2. According to the problem statement, the diffusion process continuously occurs in both subsystems, particularly at the boundary of each micropore with the general environment. In this case, the spherical surfaces of the micropores are taken as the boundary between the environments: the bulk environment of the crystal and the environment inside the micropores of the sample. We will characterize the concentration of the working agent in the bulk environment by the value $C(z,t)$, and the concentration inside the micropore will be characterized by the value l , where $0 \leq x \leq R$ and $0 \leq z \leq l$.

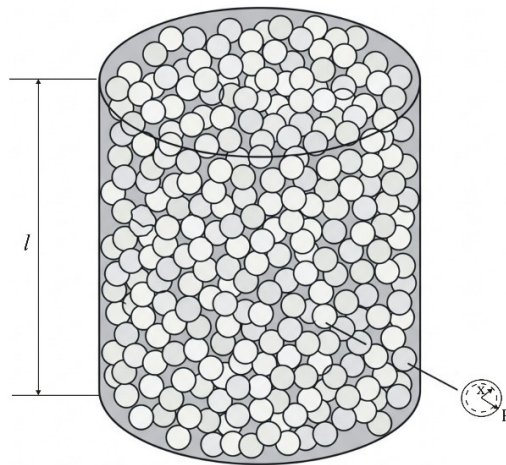


Figure 2: Model of the studied sample with pores approximated by spherical surfaces. The diffusion process occurs at the interface between the environments corresponding to the spherical surfaces of the micropores.

Since we are engaged in constructing a mathematical model of the inverse diffusion problem, our primary problem is to establish the diffusion coefficients mentioned above in both subsystems based on the experimental results available to us. These experimental results must be such that they fully describe the total concentrations of the working agent throughout the entire sample.

The current concentration in the sample at any given time is characterized by the value:

$$N(z, t) = C(z, t) + \frac{1}{R} \int_0^R Q(x, z, t) dx \quad (1)$$

that is, it is actually the sum of the concentrations in the general environment of the bulk sample, and the concentration of the adsorbed agent contained in the micropore environment.

Next, we will consider the diffusion process in both subsystems to describe the mass transfer kinetics at any time t . For this purpose, we will use general model equations that describe diffusion in the zeolite material and its micropores. These equations have the following form:

$$\frac{\partial C(z, t)}{\partial t} = \frac{D_{\text{inter}}}{l^2} \frac{\partial^2 C(z, t)}{\partial z^2} - \Gamma \frac{D_{\text{intra}}}{R^2} \frac{\partial Q(x, z, t)}{\partial x}, \quad (2)$$

$$\frac{\partial Q(x, z, t)}{\partial t} = \frac{D_{\text{intra}}}{R^2} \left[\frac{\partial^2 Q(x, z, t)}{\partial x^2} + \frac{2}{x} \frac{\partial Q(x, z, t)}{\partial x} \right], \quad (3)$$

where $D_{\text{inter}}=D_0$, $D_{\text{intra}}=D_1$ are the aforementioned diffusion coefficients that need to be found, Γ - it is a dimensionless coefficient that accounts for the porosity of the sample medium. As can be seen from equations (2) and (3), they are interconnected, indicating that they form a system of self-consistent partial differential equations. On the other hand, this necessitates checking the convergence of the solutions of both equations and the computational complexity when implementing a numerical approach. Without loss of generality, we will take the first equation as the main one – it describes the diffusion kinetics in the bulk environment. Then the second equation will act as a correction for the presence of processes describing the diffusion kinetics in micropores.

2.3. Numerical implementation of the mathematical model of diffusion in microporous samples. Finite difference scheme for the inverse diffusion problem with a complete set of data on spatial and temporal concentration distributions in the sample

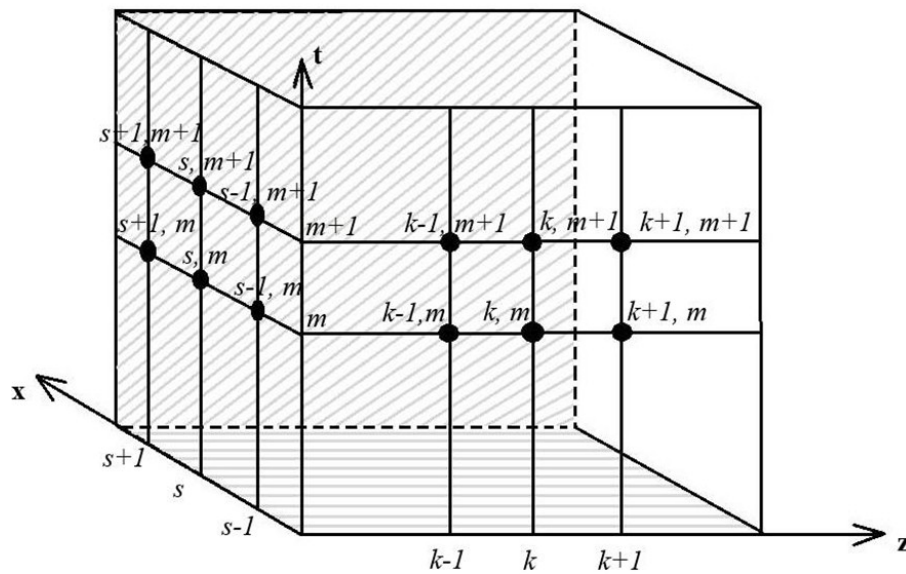


Figure 3: Three-dimensional grid and the difference scheme implemented on it.

Let's start with the development of a numerical mathematical model for the inverse diffusion problem. In this case, we will use two approaches. In the first approach, we consider that we have all concentration distributions available at certain time intervals, as well as concentration gradients in the bulk crystal environment and inside the micropore. The second approach implies the absence of some information about the concentration of the working agent in the micropores, but this information can be restored by averaging the concentration value inside each individual micropore. In each of these cases, we will only need equations (2) and (3).

We will work in a three-point approximation of derivatives, according to which all derivatives are replaced by finite difference quantities. For example, consider a function of two variables $f(x, t)$. The approximation of its first and second derivatives with respect to the variable x is as follows:

$$\begin{aligned}\frac{\partial f(x, t)}{\partial x} &\rightarrow \frac{f_{i+1} - f_i}{\Delta x_i} = \frac{f_{i+1} - f_i}{h}, \\ \frac{\partial^2 f(x, t)}{\partial x^2} &\rightarrow \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x_i^2} = \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}.\end{aligned}\quad (4)$$

In expressions (4), the quantity $h = x_{i+1} - x_i$ - is the unit step of the linear grid, and "i" is an integer, that numbers the nodes of this grid. Let us now apply relations (4) to equations (2) and (3), replacing all derivatives in them with difference quantities. We will have:

$$\begin{aligned}\frac{\partial C(t, z)}{\partial t} &= \frac{C_{k+1, s, m} - C_{k, s, m}}{\Delta t_k} = \frac{C[k+1, s, m] - C[k, s, m]}{\Delta t_k}, \\ \frac{\partial Q(t, x, z)}{\partial x} &= \frac{Q_{k, s+1, m} - Q_{k, s, m}}{\Delta x_s} = \frac{Q[k, s+1, m] - Q[k, s, m]}{\Delta x_s}, \\ \frac{\partial^2 C(t, z)}{\partial z^2} &= \frac{C[k, s, m-1] - 2C[k, s, m] + C[k, s, m+1]}{2(z_m)^2}, \\ \frac{\partial Q(t, x, z)}{\partial t} &= \frac{Q_{k+1, s, m} - Q_{k, s, m}}{\Delta t_k} = \frac{Q[k+1, s, m] - Q[k, s, m]}{\Delta t_k}, \\ \frac{\partial^2 Q(t, x, z)}{\partial x^2} &= \frac{Q[k, s-1, m] - 2Q[k, s, m] + Q[k, s+1, m]}{(\Delta x_s)^2}, \\ \frac{1}{x} \frac{\partial Q(t, x, z)}{\partial x} &= \frac{Q[k, s+1, m] - Q[k, s, m]}{s(\Delta x_s)^2}.\end{aligned}\quad (5)$$

If we substitute the result (5) into the original equations (2) and (3), after performing simple transformations, we will have:

$$\begin{aligned}&\frac{C[k+1, s, m] - C[k, s, m]}{\Delta t_k} = \\&= \frac{D_0}{l^2} \frac{C[k, s, m-1] - 2C[k, s, m] + C[k, s, m+1]}{(\Delta z_m)^2} - \Gamma \frac{D_1}{R^2} \frac{Q[k, s+1, m] - Q[k, s, m]}{\Delta x_s}, \\&\frac{Q[k+1, s, m] - Q[k, s, m]}{\Delta t_k} = \\&= \frac{D_1}{R^2} \left(\frac{Q[k, s-1, m] - 2Q[k, s, m] + Q[k, s+1, m]}{(\Delta x_s)^2} + \frac{2Q[k, s+1, m] - 2Q[k, s, m]}{s(\Delta x_s)^2} \right).\end{aligned}\quad (6)$$

The difference scheme, which is defined according to relations (6), is built on a three-dimensional grid, which corresponds to the discretization of equations (2) and (3) with respect to the coordinates x , z , and the time variable t . As a result, the spatial domain on which the difference scheme (6) is defined is as follows:

$$\Omega = \begin{cases} T \cup X \cup Z, T = \{k\Delta t_k, k = 1..k_{\max}\}; \Delta t_k = t_{\max} / k_{\max} = \Delta t_k = t[k+1] - t[k]; \\ X = \{s\Delta x_s, s = 1..s_{\max}\}; \Delta x_s = X_{\max} / s_{\max} = X[m+1] - X[m]; X_{\max} = 1; \\ Z = \{m\Delta z_m, m = 1..m_{\max}\}; \Delta z_m = Z_{\max} / m_{\max} = Z[m+1] - Z[m]; Z_{\max} = 1, \end{cases} \quad (7)$$

$$(k; s; m) \in Z^+.$$

we will also assume that: $k_{\max} = s_{\max} = m_{\max} = 100$, and the time interval can be obtained from experimental data: $T = (0, t_{\max})$. The resulting difference scheme and three-dimensional grid can be visualized as shown in Figure 3.

Within each node $[k, s, m]$ of the three-dimensional grid, the difference scheme (6) represents a system of two equations for determining the diffusion coefficients D_1 and D_2 . This system of equations can be reduced to the following form:

$$\begin{cases} a_{ksm}D_0 + b_{ksm}D_1 = c_{ksm}; \\ d_{ksm}D_1 = e_{ksm}, \end{cases} \quad (8)$$

where

$$\begin{aligned} a_{ksm} &= \frac{C[k, s, m-1] - 2C[k, s, m] + C[k, s, m+1]}{(l\Delta z_m)^2}; \quad b_{ksm} = -\frac{\Gamma}{R^2} \frac{Q[k, s+1, m] - Q[k, s, m]}{\Delta x_s}; \\ c_{ksm} &= \frac{C[k+1, s, m] - C[k, s, m]}{\Delta t_k}; \\ d_{ksm} &= \frac{1}{R^2} \left(\frac{Q[k, s-1, m] - 2Q[k, s, m] + Q[k, s+1, m]}{(\Delta x_s)^2} + \frac{2Q[k, s+1, m] - 2Q[k, s, m]}{s(\Delta x_s)^2} \right); \\ e_{ksm} &= \frac{Q[k+1, s, m] - Q[k, s, m]}{\Delta t_k}. \end{aligned} \quad (9)$$

From the system of equations (8) we now directly obtain:

$$D_0 = \frac{c_{ksm}}{a_{ksm}} - \frac{b_{ksm}}{a_{ksm}} D_1 = \frac{c_{ksm}}{a_{ksm}} - \frac{b_{ksm}e_{ksm}}{a_{ksm}d_{ksm}}; \quad D_1 = \frac{e_{ksm}}{d_{ksm}}. \quad (10)$$

The diffusion coefficient values found at each node $[k, s, m]$ of the discrete grid allow, in an iterative approach, to move to any of these nodes:

$$\begin{aligned} &[k-1, s, m]; [k+1, s, m]; [k, s-1, m]; [k, s+1, m]; [k, s, m-1]; [k, s, m+1]; \\ &[k-1, s-1, m]; [k-1, s+1, m]; [k+1, s-1, m]; [k+1, s+1, m]; \\ &[k-1, s-1, m-1]; [k-1, s-1, m+1]; [k-1, s+1, m-1]; [k+1, s+1, m+1] \end{aligned} \quad (11)$$

As a result, it becomes clear that each node will be accounted for k, s, m times in each direction of the discrete grid. Thus, the diffusion coefficient values obtained from a direct pass of the grid will be as follows:

$$D_0 = \frac{1}{k!s!m!} \sum_{k=1}^{k_{\max}} \sum_{s=1}^{s_{\max}} \sum_{m=1}^{m_{\max}} \left(\frac{c_{ksm}}{a_{ksm}} - \frac{b_{ksm}e_{ksm}}{a_{ksm}d_{ksm}} \right); \quad D_1 = \frac{1}{k!s!m!} \sum_{k=1}^{k_{\max}} \sum_{s=1}^{s_{\max}} \sum_{m=1}^{m_{\max}} \frac{e_{ksm}}{d_{ksm}}, \quad (12)$$

where the presence of the multiplier $1/k!s!m!$ solves the problem of multiple accounting for the same nodes of the difference scheme.

2.4. Difference scheme for the inverse diffusion problem in the absence of a dataset of spatial and temporal concentration distributions in the micropores of the sample

In many cases, the concentration values inside micropores are difficult to determine, or they were not directly the goal of the experiment. In this case, the system of diffusion equations at the macro- and micro-levels can also be replaced by a difference scheme. However, it is necessary to

approximate the concentration values inside the micropores with their averaged values over the sample volume. We again arrive at the following system of equations:

$$\begin{cases} \frac{\partial C(z,t)}{\partial t} = \frac{D_0}{l^2} \frac{\partial^2 C(z,t)}{\partial z^2} - \Gamma \frac{D_1}{R^2} \frac{\partial Q(x,z,t)}{\partial x}; \\ \frac{\partial Q(x,z,t)}{\partial t} = \frac{D_1}{R^2} \left[\frac{\partial^2 Q(x,z,t)}{\partial x^2} + \frac{2}{x} \frac{\partial Q(x,z,t)}{\partial x} \right]. \end{cases} \quad (13)$$

According to Lagrange's theorem for the equation describing the substance balance in the sample, we have:

$$M(t,z) = C(t,z) + \int_0^{\bar{X}} Q(t,x,z) dx = C(t,z) + Q(t,\bar{X},z) \bar{X} \quad (14)$$

and in this way, we got rid of the variable x by replacing the concentration inside the micropore with the averaged value over its radius \bar{X} .

Let us now consider an auxiliary system of diffusion equations, homologous to the system (13):

$$\begin{cases} \frac{\partial C(z,t)}{\partial t} = \frac{D_0}{l^2} \frac{\partial^2 C(z,t)}{\partial z^2} - \Gamma \frac{D_1}{R^2} \frac{\partial Q(x,z,t)}{\partial x}; \\ \int_0^{\bar{X}} \frac{\partial Q(x,z,t)}{\partial t} dx = \frac{D_0}{l^2} \int_0^{\bar{X}} \frac{\partial^2 Q(x,z,t)}{\partial z^2} dx - \Gamma \frac{D_1}{R^2} \int_0^{\bar{X}} \frac{\partial C(z,t)}{\partial x} dx. \end{cases} \quad (15)$$

where the second equation is averaged over the radius x .

After simplifications using Lagrange's theorem and using the relation (14), we will have equivalent equations for the averaged value of the total concentration. They are already partial differential equations only with variables t and z :

$$\begin{cases} \frac{\partial M(z,t)}{\partial t} = \frac{D_0}{l^2} \frac{\partial^2 M(z,t)}{\partial z^2} - \Gamma \frac{D_1}{R^2} M(z,t); \\ \frac{\partial M(z,t)}{\partial t} = \frac{3(D_0 + D_1)}{R^2} \frac{\partial^2 M(z,t)}{\partial z^2}. \end{cases} \quad (16)$$

Using relations (4), the following difference scheme is obtained:

$$\begin{cases} A_{ksm} = D_0 B_{ksm} + D_1 C_{ksm}; \\ D_{ksm} = (D_0 + D_1) E_{ksm}, \\ A_{ksm} = \frac{M[k,s,m]}{\Delta t_k}; B_{ksm} = \frac{M[k,s,m-1] - 2M[k,s,m] + M[k,s,m+1]}{(l \Delta z_m)^2}; \\ C_{ksm} = -\Gamma \frac{M[k,s,m]}{R^2}; D_{ksm} = \frac{M[k+1,s,m]}{\Delta t_k}; \\ E_{ksm} = \frac{3(M[k,s,m-1] - 2M[k,s,m] + M[k,s,m+1])}{(R \Delta z_m)^2}. \end{cases} \quad (17)$$

The resulting iterative loop is only executed along the variable m . Indices k, s can be omitted, since they play the role of silent indices in the difference scheme. As a result, we again obtain a system of linear equations with respect to the diffusion coefficients and at each node of the one-dimensional discrete grid:

$$\Omega = (\{m \Delta z_m, m = 1..m_{\max}\}; \Delta z_m = Z_{\max} / m_{\max} = Z[m+1] - Z[m]; Z_{\max} = 1, m \in Z^+). \quad (18)$$

In relations (16), (17), are the values of total concentrations, which are most often obtained experimentally as a result of direct measurements. Then the solutions of system (17) are as follows:

$$D_0 = \frac{A_{ksm}}{B_{ksm}} - \frac{C_{ksm}D_{ksm}}{E_{ksm}(A_{ksm} - C_{ksm} + B_{ksm})}; D_1 = \frac{D_{ksm}B_{ksm}}{E_{ksm}(A_{ksm} - C_{ksm} + B_{ksm})}. \quad (19)$$

3. Development of a software system architecture performing mathematical modeling of the diffusion process and identification of working agent parameters from experimental parameters

An important aspect of working with input data used in the implementation of the mathematical model of the inverse problem is the format of this data. Since we will use the Wolfram Mathematica environment in our software system, where programming is done directly using a C-like language, it is necessary to provide the ability to read data line by line. This is also due to the fact that the data from experimental studies, which we use as input data, are in the form of two columns. For example, the input data for concentration are given in the form $c(a)=b$, where a and b are the corresponding columns of a file with the extension .txt, .doc, .rtf. In order for our final software system to work with this data, it is necessary to format the text format of the input data into a supported MS-DOS digital format. This can be done by converting this data into a format with the .dat extension, with support for reading data using the following commands: $c \rightarrow \tilde{c} = CForm(c); DosTextFormat \rightarrow True$. This will allow the input data to be submitted in floating-point format and read from the input file line by line.

Given the direct structure of the mathematical models of the direct and inverse problems and the difference schemes that implement them, the architecture of the software system and the client-system architecture were built.

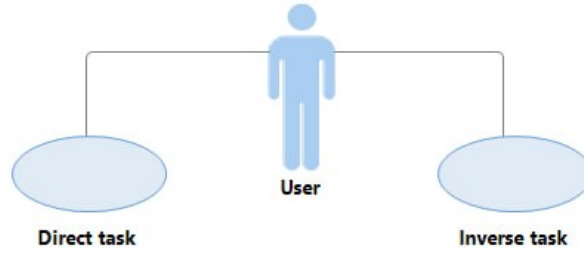


Figure 4: Software system architecture diagram without branching.

Figure 4 shows the software system architecture diagram. According to it, the user can choose at the input to work with the inverse or direct problem for mathematical diffusion models. The program block of the direct and inverse problems was developed separately and has a different structure in accordance with the tasks that the components of the software system solve. The detailed architecture of each of the program system – its use case diagram blocks is shown in Figure 5.

In accordance with the developed architecture of the software system for the mathematical model of the inverse problem, the following actions are provided:

- loading experimental input data and, if necessary, formatting them into .dat format with floating point;
- entering geometric parameters of the sample;
- visualization of experimental data;
- identification of diffusion parameters from the inverse problem;
- visualization of the time dependence of diffusion coefficients.

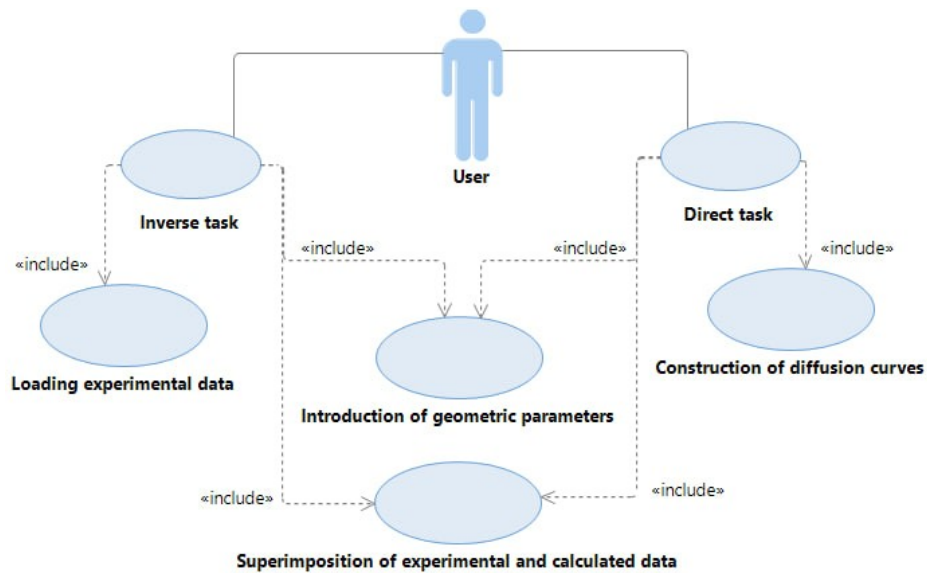


Figure 5: Use case diagram of the software system with a representation of the user interface capabilities.

A more detailed specification of this software module is shown in Figure 6a. This figure most fully describes the architecture of each of its components and demonstrates its functionality, designed for a variety of tasks.

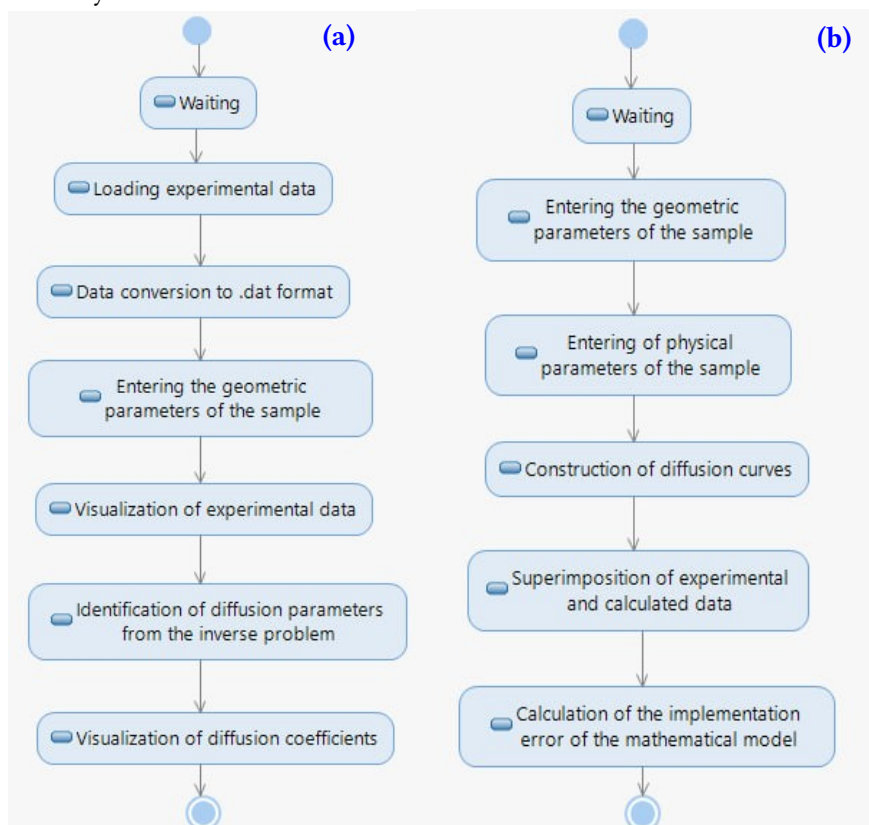


Figure 6: Detailed architecture of the software module implementing the mathematical model of the inverse problem (a), and the software module implementing the mathematical model of the direct problem (b).

Further, the architecture of the program block related to the implementation of direct mathematical models was developed. During the development of the architecture, the key issues were considered to be ensuring the ability to effectively change the input parameters of the mathematical model, as well as functionality providing visualization of the results obtained, their comparison with each other in order to ensure verification. In accordance with the developed architecture of the software system for the mathematical model of the direct problem, the following actions are provided:

- entering the geometric parameter of the sample;
- entering the physical parameter of the sample;
- construction of diffusion curves;
- overlaying (comparing) experimental calculated and their interpolation;
- calculations of the accuracy of the implementation of the mathematical model.

4. Practical implementation of a software system for direct and inverse problems of mathematical modeling of the diffusion process in microporous samples

4.1. Working with experimental diffusion curves, obtaining diffusion coefficients at arbitrary time intervals

The entire construction of the information system and its components was carried out in the Wolfram Mathematica 12 environment. At the first stage of developing work with the developed information system, preliminary preparation and processing of input data corresponding to the experimental study of directly developed samples are performed. The developed functionality of the program system block, which is designed to work with data obtained from the inverse problem of the diffusion mathematical model and process experimental data, is as shown in Figure 7.

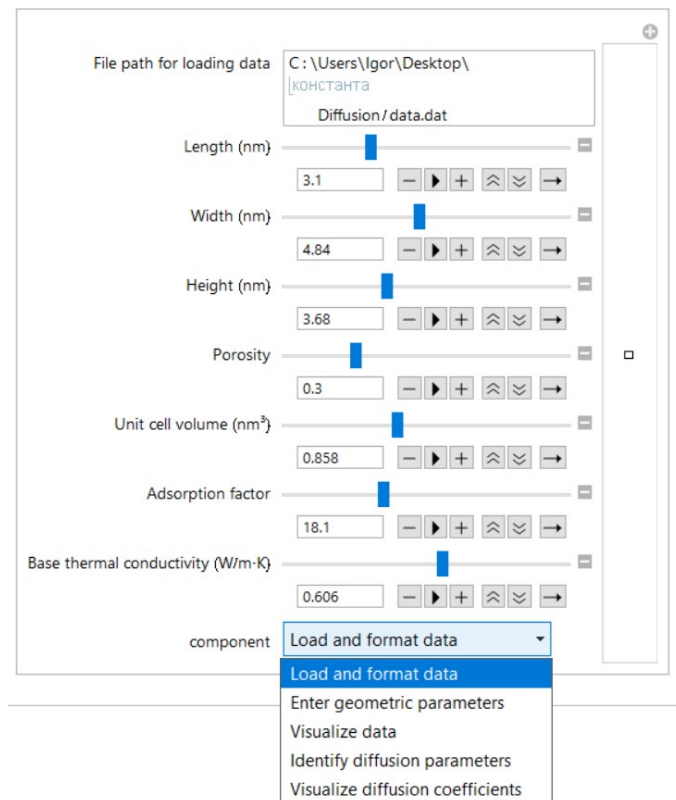


Figure 7: Example of working with a software block designed for the inverse diffusion problem.

Next, Figure 8a, b shows examples of concentration curves obtained as a result of direct measurements for an experimentally created zeolite sample, representing the results of the software system block execution. The construction of concentration curves was carried out using the input block of the software system with the use of directives of the List Plot and List Line Plot functions after their preliminary processing. These necessary data were taken directly from the list of experimental papers [13-19].

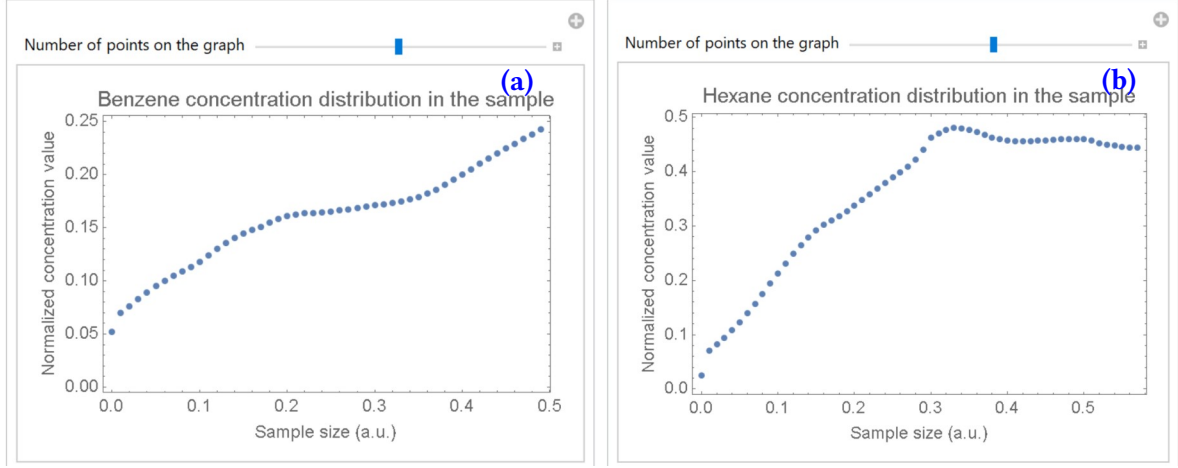


Figure 8: Example of experimentally realized concentration distribution in a sample of benzene a) and hexane b).

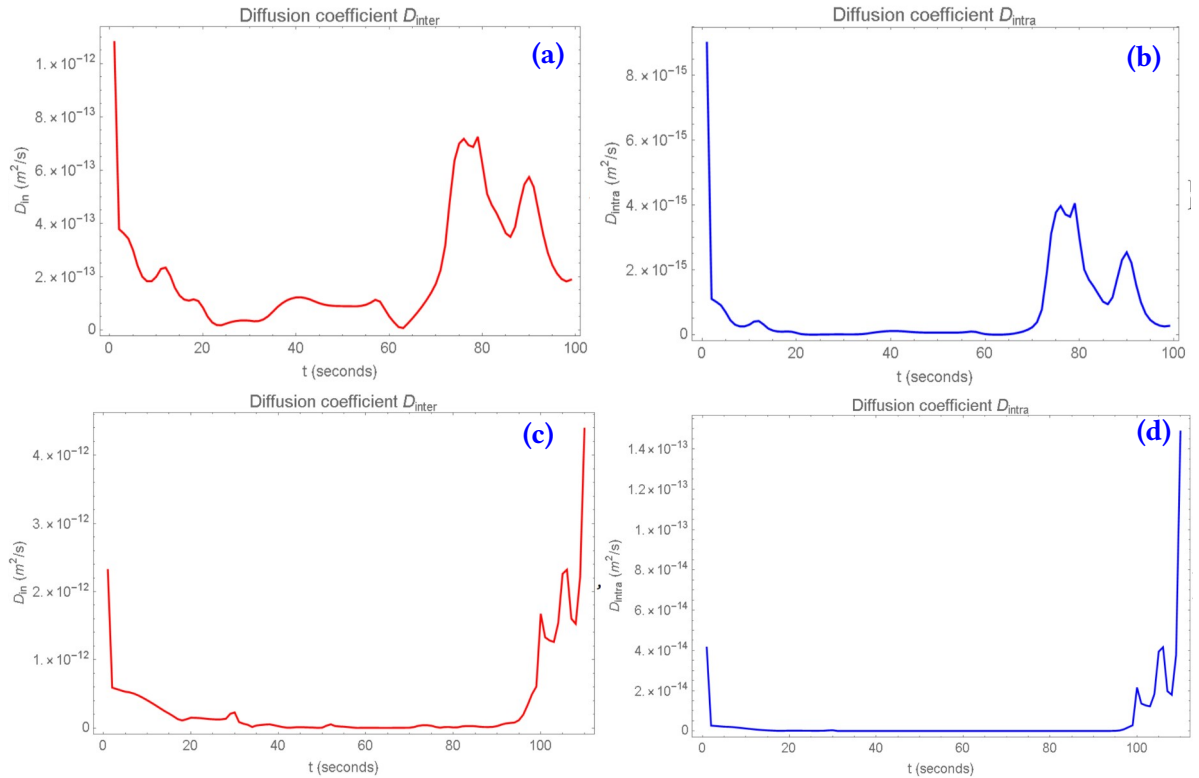


Figure 9: Dependencies of diffusion coefficients D_{inter} and D_{intra} on time t for benzene a), b) and hexane c), d).

After processing the obtained information about concentration, the distribution dependence for benzene in the sample is obtained, for convenience, the sample sizes and concentration values are presented in relative units. Similar preparatory actions for processing the experimentally obtained hexane diffusion concentration on an analogous sample were performed.

At the input data processing stage, it is possible to adjust the input number of concentration curve points, which greatly facilitates working with cases where we have a very large amount of input data with a given static deviation. This allows, during the final processing of experimental data, using only the input block of our developed software system, to apply data approximation using splines or interpolation polynomials, solely at the user's discretion, which is directly implemented in the Wolfram Mathematica software environment itself.

For the experimental data, the processing of which was performed using the software block presented in the previous subsection of the thesis, a difference scheme for the inverse diffusion problem was applied, given by relations (9), (10), (12), (19). As a result, the sought values of diffusion coefficients $D_{\text{inter}}=D_0$ and $D_{\text{intra}}=D_1$ are obtained. The dependencies of the diffusion coefficients for benzene and hexane on time, calculated from the difference scheme, are shown in Figure 9a, b, c, d. As can be seen from Figure 9, the developed mathematical models for the inverse diffusion problem allow visually establishing differences in the dependencies of diffusion coefficients of different types of volatile agents (benzene and hexane, respectively), as well as comparing their numerical values.

4.2. Verification and validation of the mathematical model of the inverse diffusion problem

To verify the developed mathematical models and the developed software, modeling of various types of samples was performed based on the obtained diffusion parameters of benzene and hexane, which were obtained from other samples of the same type and other works. With known diffusion coefficients, relations (8), (9) and (17) represent a grid problem for the direct mathematical model of diffusion and allow calculations of concentration distributions of benzene and hexane and comparison of the obtained results with experimental ones.

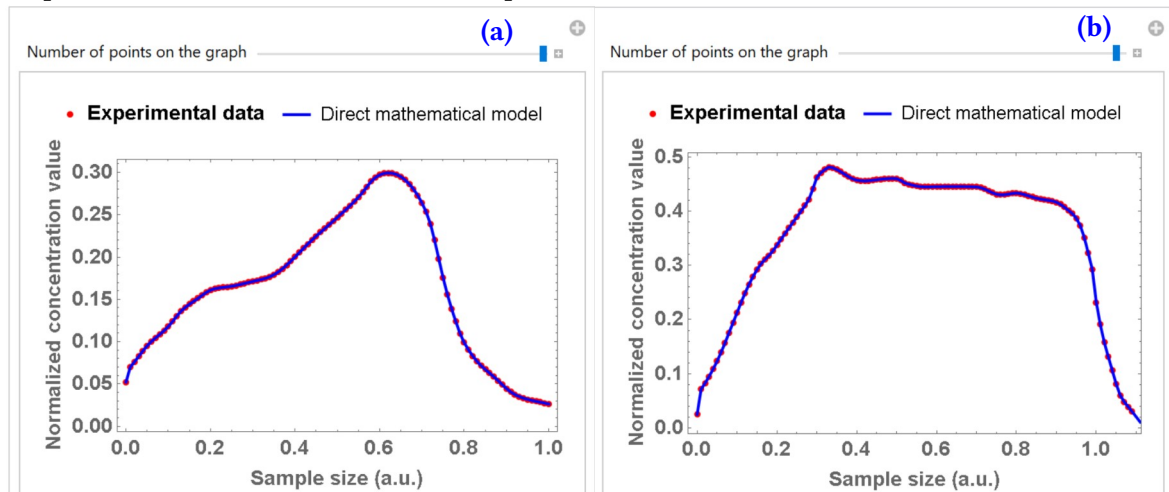


Figure 10: Concentration profiles calculated from the direct mathematical model of diffusion and their comparison with experimental data for benzene (a) and hexane (b).

Figure 10 shows, for comparison, the calculated concentration curves of benzene and hexane from papers [13-16, 18] and their experimental data, while the diffusion coefficients were calculated based on experimental data taken from a completely different papers [17, 19]. As can be seen from the figures presented, the identified diffusion parameters provide good agreement of the results given by the direct mathematical model of diffusion with the experiment. Thus, we can speak about the adequacy of the proposed approach to obtaining diffusion parameters and verifying the direct mathematical model of mass transfer, which allows extending the developed methodology to a whole range of typical samples, the results of mathematical modeling for which are not yet known. It is also possible to assert the possibility of identifying diffusion parameters for various volatile agents based on collecting experimental data on their concentration profiles.

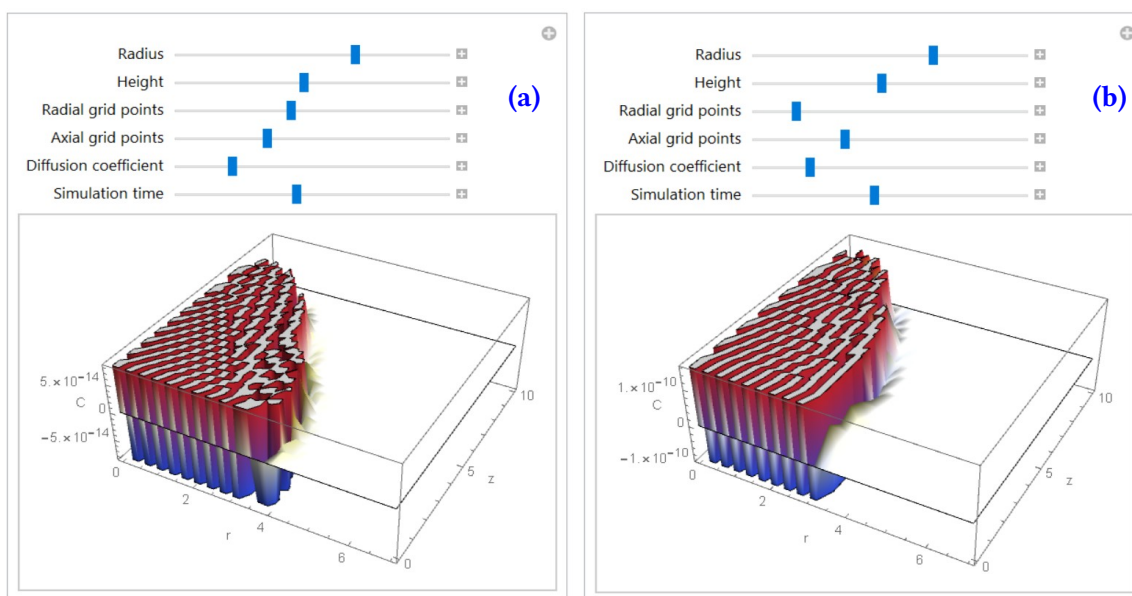


Figure 11: Concentration profiles calculated from the direct mathematical model of diffusion and their comparison with experimental data for benzene a) and hexane b).

The final stage of verification is the implementation of a software system block that implements the construction of a spatial dependence of concentration for the mass transfer process in a cylindrical sample. The software implementation of this process is shown in Figure 11. This software system block is implemented in such a way that in direct modeling, it is possible to use diffusion coefficients obtained from the inverse problem, as well as select the necessary geometric and physical parameters of the sample. As a result, an algorithmized mathematical model is obtained with the possibility of integrative change of its parameters and implemented possibility of 3D visualization of results, in particular, the presented results demonstrate differences between the spatial concentration distributions of benzene (a) and hexane (b).

5. Conclusions

The main practical results presented in this work are as follows. Mathematical models corresponding to the direct and inverse diffusion problems in microporous samples with cylindrical symmetry have been developed. Finite-difference schemes approximating them as grid problems have been developed for the obtained mathematical models. By algorithmizing finite-difference schemes in the Wolfram Mathematica software environment, a software system has been developed, which was applied to identify diffusion coefficients based on the analysis of arrays of experimentally obtained data on the concentration distribution of benzene and hexane. The verification of the developed mathematical models was carried out by applying the parameters obtained from the inverse diffusion problem to modeling concentration distributions in other samples with comparison of the model results with experimental ones. In addition, software components have been developed that allow performing spatial visualization of the concentration of volatile compounds in cylindrical samples and changing their precision parameters. For the developed software components, a unifying architecture of the software complex has been developed, which provides, in addition to working with the main components that implement the direct and inverse diffusion problems, the ability to perform preliminary processing of input data, compare numerical and visualized results. The developed human-machine interface facilitates working with the components of the software complex, allowing to change the input parameters of mathematical models and export the obtained results in both numerical and graphical formats.

Declaration on Generative AI

The authors have not employed any Generative AI tools.

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