Software complex for mathematical modeling of diffusion processes in various zeolite samples*

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Abstract

The architecture and structure of a complex of software system components designed to implement mathematical modeling of diffusion transfer processes in various samples of microporous materials, specifically zeolites, has been developed. This problem was solved in several stages. First, mathematical models of mass and heat transfer in zeolites were constructed and generalized for the case where the studied samples have an arbitrary number of layers and variable geometric parameters. For the developed mathematical models, presented in the form of boundary value problems and boundary conditions, their approximation by grid finite-difference schemes suitable for their further algorithmization was performed. At the next stage, the software implementation of each component of the software complex was carried out using the Wolfram Mathematica environment and programming language. In the final stage, the architecture of the software complex was developed, which connects all its developed components, and also provides user interaction with the software system and allows them to vary the input parameters of the implemented mathematical models. Verification of the developed mathematical models and the operation of the software system was carried out by testing the operation of all its components and using typical parameters of zeolite samples. The developed software complex meets the needs of both researchers and engineers directly working in this subject area. The functionality and tools of the software complex can be further easily modified and complicated according to emerging needs.

Keywords

Software complex, mathematical model, Wolfram Mathematica

1. Introduction. Domain analysis

In recent years, there has been an active infiltration of methodologies and approaches developed within information technology, particularly software engineering, into science and technology in general. For example, mathematical modeling methods combined with object-oriented programming tools enable the study of new materials, micro- and nanostructures at a completely different level of perception and visualization. The development of nanoscale samples with predetermined properties and geometries requires not only the physicochemical properties of the starting materials but also the application of complex software systems that control these processes and minimize human influence.

Diffusion processes related to mass and heat transfer kinetics constitute an actively and rapidly modernizing part of modern technologies. Functional materials of amorphous, crystalline, or semiconductor origin can act as working agents for the transport of various substances (hydrocarbon molecules, inert gases, water vapor) [1-3], electrons, and quasiparticles [4-6]. Working with such functional materials is quite complex and requires the comprehensive

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application of modern methods of spectroscopy, materials science, and especially information technology. In particular, the growth of microstructures of this type requires significant control over their geometric and spatial dimensions, which are actually the determining factor of their properties. In this regard, a whole direction has emerged in software engineering related to the subject area of developing software systems that allow pre-varying the properties and dimensions of microsystems [7, 8]. This is an extremely important and useful direction, as it allows engineers and experimental researchers to select the necessary physical and geometric parameters of microstructures and their systems for their tasks using appropriate software [9-11]. It also significantly saves costs, as growing crystalline structures with predetermined parameters using molecular beam epitaxy or ion implantation methods amounts to sums on the order of several million euros [12-14].

The development of mathematical models for diffusion processes has a rather long and complex history. It has its roots in research at the beginning of the 20th century by scientists in the fields of mathematical physics and materials science. These models were mostly analytical and did not have a significant impact on the development of technologies. Everything changed in the 60-70s of the last century when scientists from the Glushkov Institute of Cybernetics managed to perform simulation and numerical modeling of diffusion kinetics processes in massive crystals for the first time. The results obtained, firstly, well described the experimental results, and secondly, the developed software, even within the framework of those times, could be quickly modified in the need to apply it to systems with different specifics and parameters [15]. The current state of research in this problem often lies in two competing directions. The first direction is highly specialized software that is created practically once for a specific scientific problem or task. Such software works efficiently and optimally, but it has one significant drawback. It cannot be modified for related problems, and the parameters of the input mathematical model can only be strengthened in a very narrow range in such a software system. An example of such software systems is the NextNano software package, which is updated several times a year. At the same time, the package includes a large number of software systems, of which only a small number will be useful to users. As researchers' experience shows, attempts to simultaneously use several different NextNano software systems can give radically different results, which significantly hinders the development of this subject area from the point of view of modern information technology.

One of the problems facing software engineering in this subject area is the expansion of the functionality and specifications of the software package included in this software complex. As a result, hundreds of programmers can work on such software simultaneously, who are involved in both the development of mathematical models and the writing of the final code that implements the models [16-18].

In the proposed paper, the task is set to build mathematical models of diffusion transfer processes in complex multilayer samples created from microporous functional materials: zeolites and silica gel. In particular, similar problems were mentioned in papers [19,20]. To implement these mathematical models, their representation in the form of grid problems approximating the resulting boundary value problems with finite difference schemes will be performed. For user convenience, a convenient human-machine interface and software system architecture have been developed. The developed information system will be an interconnected software complex that allows you to quickly select the necessary dimensional and physical parameters of the studied samples, obtain the necessary numerical values provided by mathematical models, and, most importantly, interactively visualize the results of mathematical modeling. This software system will have a wide purpose: both for specialists engaged in direct research and for engineers, the functionality of the system will allow for its further improvements and variability.

2. Mathematical models applied to modeling diffusion processes

From the point of view of developing mathematical models of diffusion, the following is the basic model [9-11]. It is assumed that the diffusion process has established itself throughout the continuum of the studied sample, while the kinetics of diffusion are characterized by the dynamics of the process only at the boundaries of the medium of the zeolite crystalline material and the micropores contained therein. In this case, the mathematical model of diffusion is expressed by a self-consistent system of partial differential equations, which in the general case has the following form

$$\begin{aligned} &\frac{\partial c(z,t)}{\partial t}+\frac{\partial a(z,t)}{\partial t}+\upsilon\frac{\partial c(z,t)}{\partial z}=D_{inter}\frac{\partial^2 c(z,t)}{\partial z^2};\\ &\frac{\partial a(z,t)}{\partial t}=\beta\left[c(z,t)-c_{eq}(a)\right]. \end{aligned} \tag{1}$$

The first of the equations in system (1) is used to describe the kinetics of diffusion throughout the body of the sample, and the second equation describes the diffusion process of volatile particles through the boundary of micropores with the material medium of an arbitrary zeolite. Finding any solutions, even numerical ones, of system (1) presents significant difficulties. To this end, in paper [9], diffusion was assumed to be an equilibrium process, which was ensured by the condition:

$$c_{eq}(a)=a/b(a_{full}-a) \tag{2}$$

where the parameters a, b, a_{full} were assumed to be dependent on the current concentration of the volatile agent, and in general form they were certainly complex nonlinear functions of temperature T, according to the so-called Langmuir isotherm, which considers the non-ideality of the gas, the size of the molecules and the interaction between them and with the crystal lattice of the sample as a limiting factor. In addition, the flow rate of gas through the sample was assumed to be adiabatic, according to the well-known relation:

$$\upsilon=\sqrt{\frac{C_{mP}R}{C_{mV}T}} \tag{3}$$

In papers [10, 11], a number of approximations were made that simplified the mathematical module of diffusion (1). In particular, the equilibrium condition between the diffusion flow and the sample medium was simplified and presented in the following form:

$$c_{eq}(a)=\gamma a+\varepsilon a^2 \tag{4}$$

where $\gamma=1/(ba_{full})$ is a constant value that characterizes diffusion in the so-called Henry's kinetics approximation. In this case, in expression (4), a small parameter ε, which characterizes the phase transition between the micropore medium and the sample medium, was used for the expansion. As a result, expression (4) and the original equations of the mathematical model are significantly simplified, it is possible to obtain their analytical expressions by applying the Laplace and Heaviside differential-integral transformations. The simplified mathematical model of diffusion in this case takes the following form:

$$\begin{aligned} &\frac{\partial c(z,t)}{\partial t}+\frac{\partial a(z,t)}{\partial t}+\upsilon\frac{\partial c(z,t)}{\partial z}=D_{inter}\frac{\partial^2 c(z,t)}{\partial z^2};\\ &\frac{\partial a(z,t)}{\partial t}=\beta\left[\gamma a(z,t)+\varepsilon a^2(z,t)\right]. \end{aligned} \tag{5}$$

For the implementation of the mathematical model, in particular the numerical one, it was assumed that model (5) is characterized by the following initial conditions:

$$c(z,t)\Big|_{t=0} = c_s; a(z,t)\Big|_{t=0} = a_s \tag{6}$$

which characterize the initial concentrations in different boundary environments of the samples. In order to be able to apply the methods of integral transformations, it was also assumed that the mathematical model (5) is characterized by a set of simple interface boundary conditions, significantly simplifying the spectral problem:

$$c(z,t)\Big|_{z=0} = \omega_0(t) = \omega_0; \frac{\partial c(z,t)}{\partial z}\Bigg|_{z=\infty} = 0 \tag{7}$$

The solutions of the mathematical model (5) with initial conditions (6) and boundary conditions (7) are obtained by the method of successive iterations using stationary perturbation theory in the form of such power series—an actual expansion in a series by a small quantity ε:

$$\begin{aligned} c\left(z,t\right) &= c_0\left(z,t\right) + \varepsilon c_1\left(z,t\right) + \varepsilon^2 c_2\left(z,t\right) + ... \\ a\left(z,t\right) &= a_0\left(z,t\right) + \varepsilon a_1\left(z,t\right) + \varepsilon^2 a_2\left(z,t\right) + ..., \end{aligned} \tag{8}$$

where each of the terms in expressions (8) could be obtained in an analytical, but at the same time in a rather complex for software implementation, formulaic construction.

The mentioned mathematical model, although it is the main and basic one for describing diffusion processes in samples with micropores, nevertheless has a number of significant shortcomings that do not allow it to be applied to the description of mass transfer processes in multilayer samples. These shortcomings include:

- the use of approximations and perturbation theory at early stages of mathematical model construction; initial conditions of the form (6) significantly impose restrictions on input data in the software implementation of the mathematical model;
- the convergence of series in expressions (8) is difficult to establish directly, although direct calculations indicate the possibility of achieving the required computational accuracy;
- boundary conditions (7) are very formal and simplified, their application to multilayer structures would have totally incorrect results.

In summary, it should be concluded that to successfully solve the problem of constructing a mathematical model of mass transfer in multilayer samples, the existing mathematical model should be significantly adjusted and improved. To do this, the following should be done: introduce more general initial conditions for the concentration in the sample and its micropores; it is necessary to completely, in a different approach, approach the derivation of boundary conditions at the boundaries of the sample layers, which relate to different types of materials, in order to more realistically describe them; for the obtained mathematical model, it is necessary to replace it with an effective difference scheme, which is not most optimally suited for the development of a software system, including on the basis of distributed and parallel computing; for a software system that implements a mathematical model, it is necessary to clearly think through its architecture and user interface. These problems are further solved sequentially in this paper.

3. Modification of mathematical models of mass transfer for the case of multilayer samples. Construction of grid finite-difference scheme

3.1. General problem statement. Mathematical model of diffusion in multilayer spherical samples

We will model the properties of diffusion processes in a spherical multilayer zeolite sample, the cross-section of which is shown in Fig. 1. In this figure, point 0 marks the center of the sample, and the coordinates $r_1, r_2, ..., r_{N-1}, r_N$ are the boundaries of the zeolite media with different porosity.

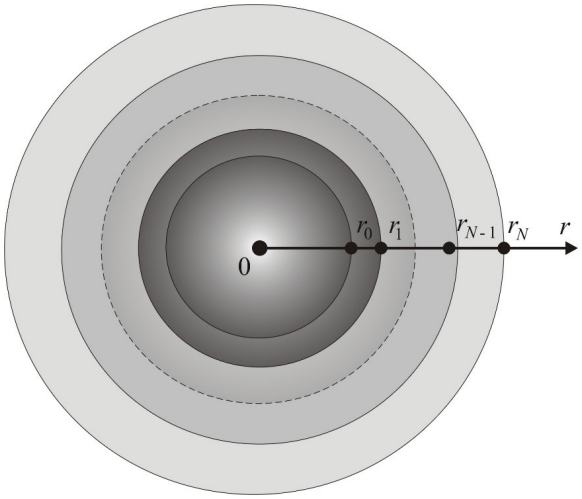

Figure 1: Cross-section of a spherical multilayer zeolite sample.

From a physical point of view, the diffusion process in the sample is complex and consists not only in the penetration of the diffusing agent into the zeolite medium. In essence, this process consists of two parts: diffusion in the intercrystalline medium of the sample and diffusion in the pores of this sample. Accordingly, the time-dependent concentrations of the dispersed substance in the intercrystalline medium and in the pores are denoted by $c(r,t)$ and $a(r,X,t)$, where $0 \le X \le \bar{X}$ and we assume that the pores in the zeolite have a spherical shape and an average radius $\bar{X}$. We will also consider that diffusion occurs for a mixture of i components that do not interact with each other. Thus, such diffusion occurs both inside the volume $4\pi r_N^3/3$ and the volume $4\pi \bar{X}^3/3$ and is most fully described by a system of self-consistent equations:

$$\begin{aligned} &\frac{\partial c(r,t)}{\partial t} = \frac{D_{\text{inter}}}{r_N^2}\frac{\partial^2 c_i(r,t)}{\partial r^2} - e_{por}\frac{D_{\text{intra}}}{\bar{X}^2}\frac{\partial a(r,X,t)}{\partial X}; \\ &\frac{\partial a_i(r,X,t)}{\partial t} = \frac{D_{\text{intra}}}{R^2}\left[\frac{\partial^2 a_i(r,X,t)}{\partial X^2} + \frac{2}{X}\frac{\partial a_i(r,X,t)}{\partial X}\right] \end{aligned} \tag{9}$$

where $D_{\text{inter}} = D_1$ and $D_{\text{intra}} = D_2$ are the diffusion coefficients of molecules of the i-th type inside the zeolite material and the pore medium, respectively. The quantity e_{por} characterizes the correction for the fact that the pores in the zeolite act as active adsorption centres. It is defined as follows:

$$e_{\text{por}} = \varepsilon_{\text{por}} / (1 - K_{\text{H}}) \tag{10}$$

where the dimensionless quantity ε_{por} determines the porosity of the zeolite medium, which is different in each layer of the sample, K_{H} – is the Henry constant.

It is considered that for concentrations outside and inside the pores, the following initial conditions are fulfilled:

$$c(r,t)\big|_{t=0} = 0; a(r,X,t)\big|_{t=0} = 0, X \in \left(0, \bar{X}\right) \tag{11}$$

To generalize the mathematical model, we assume that the zeolite system with pores is characterized by three types of boundary conditions. The first condition characterizes the constancy of concentration at the pore boundary:

$$\left.\frac{\partial a\left(r,X,t\right)}{\partial X}\right|_{X=\bar{X}} = 0 \tag{12}$$

The second boundary condition sets the adsorption equilibrium by analogy with the Langmuir condition [13]:

$$a\left(r,X,t\right)\big|_{X=\bar{X}} = \frac{K_{\text{H}} c\left(r,t\right)}{1 + K_{\text{H}} c\left(r,t\right)} \tag{13}$$

The third group of boundary conditions is designed to generalize the mathematical model for the case of an arbitrary number of different layers. They describe the equilibrium of concentrations and particle fluxes inside the layers of the zeolite sample. These boundary conditions have the following interface form:

$$\left[\begin{array}{l} c^{(m)}\left(r,t\right)\big|_{r=r_m} = c^{(m+1)}\left(r,t\right)\big|_{r=r_m}; \; m = 0, 1, 2, \ldots N \\ D^{(m)} \left.\dfrac{\partial c^{(m)}\left(r,t\right)}{\partial r}\right|_{r=r_m} = D^{(m+1)} \left.\dfrac{\partial c^{(m+1)}\left(r,t\right)}{\partial r}\right|_{r=r_m} \end{array}\right. . \tag{14}$$

3.2. Development of a finite difference scheme for the developed mathematical model. Approaches to algorithmization of the grid problem

Next, we need to obtain a finite-difference formula for the system of equations (9), which define the studied mathematical model. To do this, we will use the approximation of the first and second derivatives in the form of an approximated (right) first derivative and a three-point scheme for the second derivative. For an arbitrary function, the approximation has the following form:

$$\frac{\partial \varphi(z,t)}{\partial z} \approx \frac{\varphi_{i+1} - \varphi_i}{\Delta z}; \frac{\partial^2 \varphi(z,t)}{\partial z^2} \approx \frac{\varphi_{i-1} - 2\varphi_i + \varphi_{i+1}}{\Delta z^2} \tag{15}$$

Next, we will replace the domain of definition of the system of equations (9) with a discrete domain – a three-dimensional grid over the variables *r*, *X*, and *t*. As a result of discretizing the domain of definition for each variable, a grid with nodes is obtained, which are defined as follows:

$$\Omega_{ijk} = T_i \times X_j \times R_k = \{i\Delta t; j\Delta x; k\Delta r, i = 1..K, j = 1..L, k = 1..M\} \tag{16}$$

where $\Delta t = T / K; \Delta x = \bar{X} / M; \Delta r = R / L.$. Accordingly, here T is the magnitude of the time interval during which the process occurs, and is $R = \sum_{p=0}^{N} r_p$ the total radius of the sample.

For spherical samples, it is necessary to construct a difference scheme based on equations (9) with initial conditions (11) and boundary conditions (12), (13), (14). Using approximation (15) for equations (9), we will have:

$$\begin{aligned} &\frac{c_{i+1,j,k} - c_{i,j,k}}{\Delta t} = \frac{D_1}{r_N^2} \frac{c_{i,j,k-1} - 2c_{i,j,k} + c_{i,j,k+1}}{\Delta r^2} - e_{por} \frac{D_2}{\bar{X}^2} \frac{a_{i,j+1,k} - a_{i,j,k}}{\Delta x}; \\ &\frac{a_{i+1,j,k} - a_{i,j,k}}{\Delta t} = \frac{D_2}{R^2} \left[\frac{a_{i,j-1,k} - 2a_{i,j,k} + a_{i,j+1,k}}{\Delta x^2} + \frac{2}{\bar{X}} \frac{a_{i,j+1,k} - a_{i,j,k}}{\Delta x} \right] \end{aligned} \tag{17}$$

Next, the approximation of the initial (11) conditions gives:

$$c_{0,j,k} = 0; a_{0,j,k} = 0 \tag{18}$$

and the approximation of boundary conditions (12), (13) leads to expressions:

$$\begin{aligned} &a_{i,L,k} - a_{i,L-1,k} = 0; \\ &a_{i,L,k} = \frac{K_{\mathrm{H}} c_{i,L,k}}{1 + K_{\mathrm{H}} c_{i,L,k}}. \end{aligned} \tag{19}$$

And finally, the approximation of the interface boundary conditions (14) gives us the following expressions:

$$\begin{aligned} &c_{i,j,k} - c_{i,j-1,k} = 0; \\ &D_1^{(m)} c_{i,j,k-1} - (D_1^{(m)} + D_1^{(m+1)}) c_{i,j,k} + D_1^{(m+1)} c_{i,j,k+1} = 0. \end{aligned} \tag{20}$$

Gathering now together the approximated original equations, initial and boundary conditions (17)-(20) after transformations, the final difference scheme is obtained, implementing our mathematical model:

$$\begin{aligned} &c_{0,j,k} = 0; a_{0,j,k} = 0; \\ &a_{i,L,k} - a_{i,L-1,k} = 0; \\ &c_{i,j,k} - c_{i,j-1,k} = 0; \\ &a_{i,L,k} - (K_{\mathrm{H}} c_{i,L,k}) / (1 + K_{\mathrm{H}} c_{i,L,k}) = 0; \\ &D_1^{(m)} c_{i,j,k-1} - (D_1^{(m)} + D_1^{(m+1)}) c_{i,j,k} + D_1^{(m+1)} c_{i,j,k+1} = 0; \\ &\frac{c_{i+1,j,k}}{\Delta t} + c_{i,j,k} \left[\frac{2D_1}{(r_N \Delta r)^2} - \frac{1}{\Delta t} \right] + \frac{D_1 c_{i,j,k-1}}{(r_N \Delta r)^2} + \frac{D_1 c_{i,j,k+1}}{(r_N \Delta r)^2} - \frac{e_{por} D_2 a_{i,j,k}}{\bar{X}^2 \Delta x} + \frac{e_{por} D_2 a_{i,j+1,k}}{\bar{X}^2 \Delta x} = 0 \\ &\frac{a_{i+1,j,k}}{\Delta t} + a_{i,j,k} \left[\frac{1}{\Delta t} - \frac{2D_2}{(R\Delta x)^2} + \frac{2D_2}{\Delta x \bar{X} R^2} \right] + \frac{D_2 a_{i,j-1,k}}{(R\Delta x)^2} + \left[\frac{D_2}{(R\Delta x)^2} + \frac{2D_2}{\Delta x \bar{X} R^2} \right] a_{i,j+1,k} = 0. \end{aligned} \tag{21}$$

To algorithmize the developed grid mathematical model, we applied forward and backward substitution in the Wolfram Mathematica software environment. Backward substitution allows to efficiently obtain the solution of the grid problem (21), based on the approximated initial and boundary conditions. In this case, forward substitution is a preparatory stage in which the system is reduced to a triangular matrix form. Backward substitution is the stage of directly finding the

solution using the coefficients obtained in the first stage. In the method of modeling the diffusion process developed by us, these two stages work together: first, intermediate values are found, and then its final solution. It should also be noted that the methodology developed by us for constructing difference schemes of mathematical models and their algorithmization will also be effective in solving adjacent equations of heat conduction and diffusion, especially when using implicit schemes, such as the Crank-Nicolson method.

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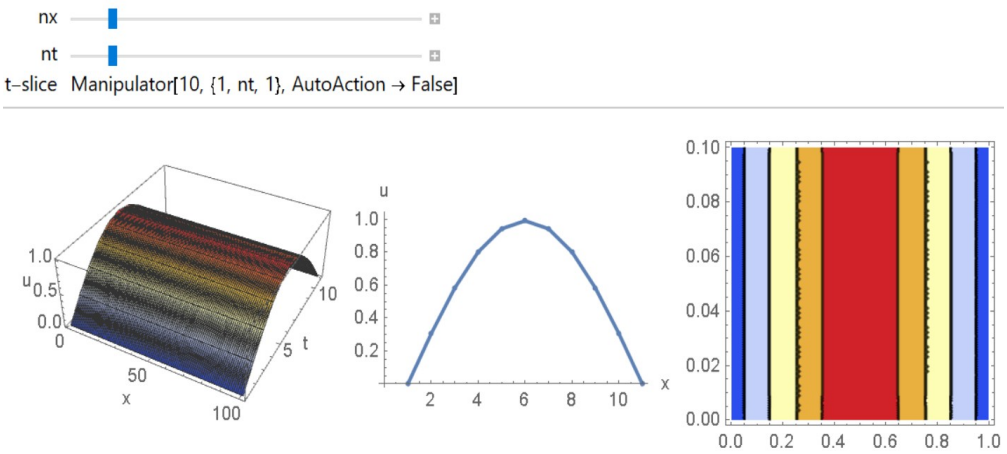


Figure 2: The result of the software system block operation for modeling the spatial dependence of the concentration distribution and its cross-sections using the Manipulate directive.

We performed a software implementation of the difference scheme block (21). It was built using the Manipulate module, which allows to arbitrarily change the sample size and the time interval in which the diffusion process occurs. An example of the operation of such a software system block is shown in Figure 2.

4. Development and design of software architecture for mathematical models of diffusion in multilayer samples

In accordance with the finite-difference form that implements mathematical models of diffusion kinetics, software was developed to realize these models. At the first stage, the software architecture was developed, which provides the most understandable interactive interaction of the user with the software system. The direct goal was to ensure variability in the user's ability to change the input parameters of the mathematical model, its physical parameters, and the geometric confinement of real studied systems. The resulting software system architecture, which is expressed in a use case diagram, is shown in Fig.ure3. It reflects the main interactions of the user with the system, defining the key scenarios of its use.

According to the developed architecture, the user does not have to directly familiarize themselves with the essence of the mathematical implementation of abstract models, since the system automates most of the calculation and data processing processes. However, restrictions were imposed in advance on the range of variable input parameters, expressing the technical side of the problem and the properties of the studied materials. These restrictions are determined based on empirical data and analytical studies, which allows to reduce the error of calculations and increase the reliability of the results. In addition, the architecture provides for the modularity of the system, which allows for its further adaptation and improvement. The main components of the system are distributed in such a way as to ensure the efficiency of computational processes, as well as convenience for the end user. An important aspect is the possibility of integration with other software systems, which expands the scope of application of the developed system.

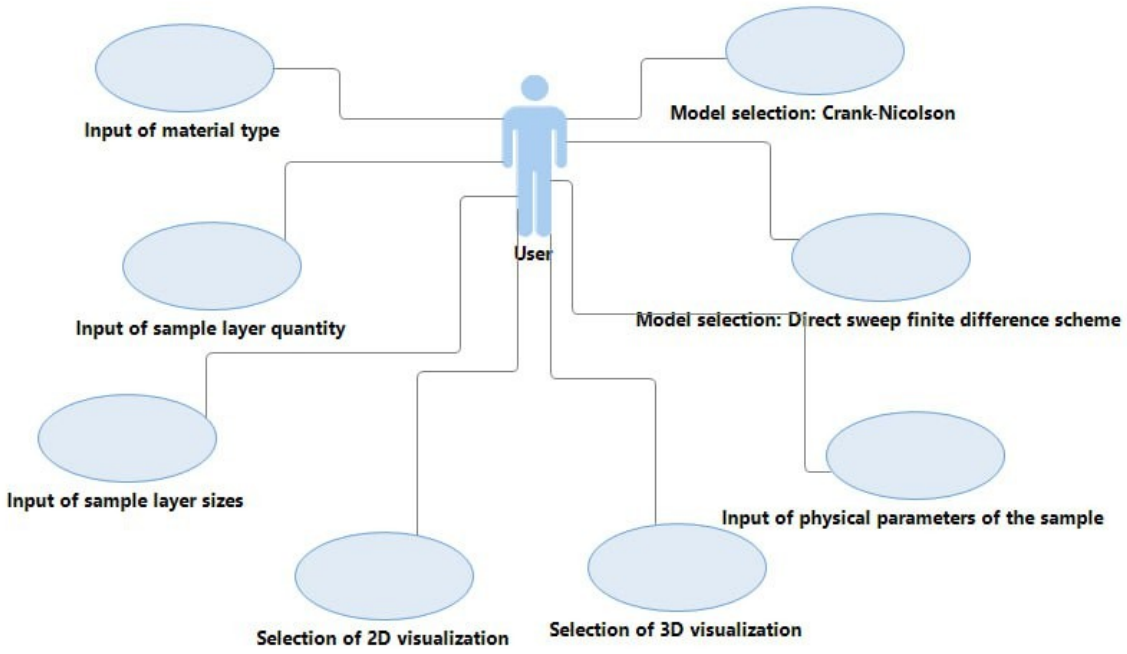


Figure 3: Use case diagram of the software system.

As a result of implementing the architecture according to the use case diagram, the software system user can perform the following actions:

- Input of sample and layer sizes and variation of their sizes within an upper limit of 10 μm;
- Input of the number of layers of the studied sample, with the upper limit of this number being limited to n=1000;
- Input of the physical parameters of the sample. In the case of choosing a sample with known physical parameters for modeling, they are already contained in the mathematical model itself;
- Input of the material type. The software system provides for operation with the following materials: zeolites ZSM-5, ZSM-9, ZSM-12, silica gel;
- Since these mathematical models were implemented in the form of Crank-Nicolson type difference schemes, the software system user can change the time parameters of the input problem and control the accuracy of the difference scheme;
- For each mathematical model and for all provided materials, the possibility of 2D and 3D visualization of spatial diffusion distributions and temperature regimes during heat and mass transfer is fully implemented.

In Figure 4 are shown the activity diagram of the developed software system, which summarizes the use case diagram presented above. According to the developed architecture, the software system, in its practical implementation, consists of two separate blocks, each of which contains four subprograms corresponding to different types of studied samples. Thus, the developed software system allows to meet the needs of a wide range of researchers. In particular, it allows to be convenient for use by scientists and engineers who work directly in the experiment and mostly need specific numerical data for comparison. In addition, the flexible visualization tools used in Wolfram Mathematica will be useful for researchers who are engaged exclusively in aspects of applied mathematical modeling of such systems and samples.

Let's analyze the principles of working with the developed software system and its components in more detail. Figure 4 shows an example of a user entering input parameters for zeolite and selecting the necessary component of the software system for its operation.

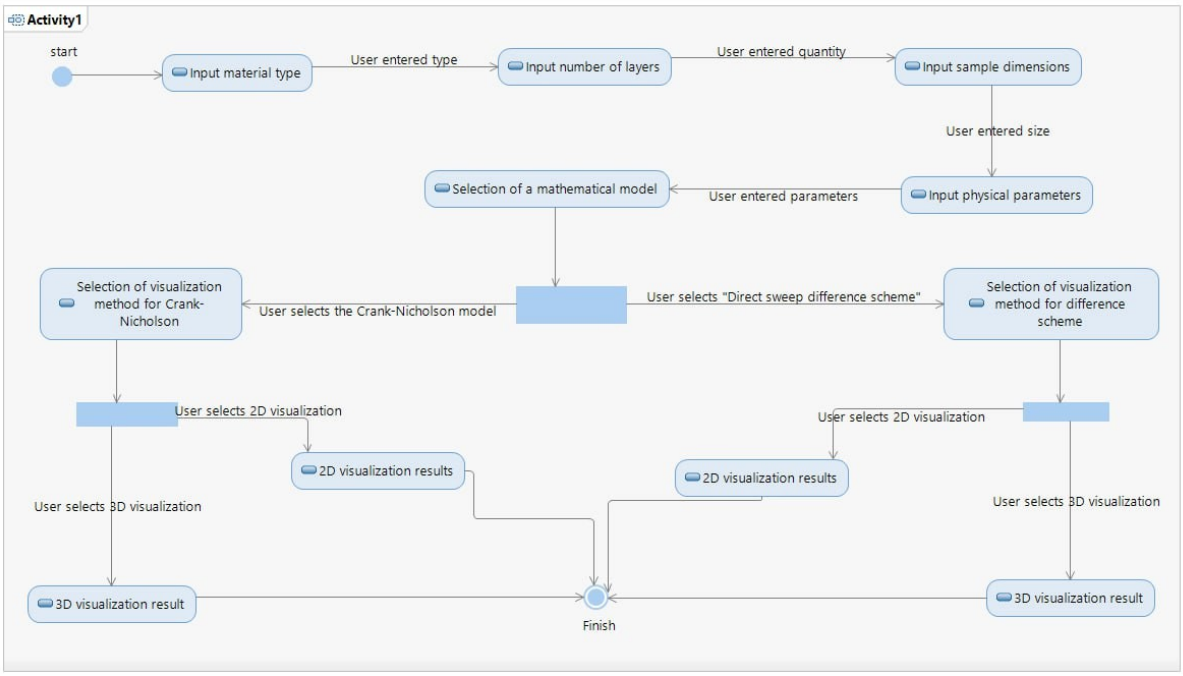


Figure 4: Activity diagram of the software system.

Work with the software system is implemented through an interface, using which the user can change the input parameters of the mathematical model, geometric and physicochemical parameters of materials using sliders. For example, the user menu for selecting sample parameters based on ZSM-5 zeolite is shown further in Figure 5.

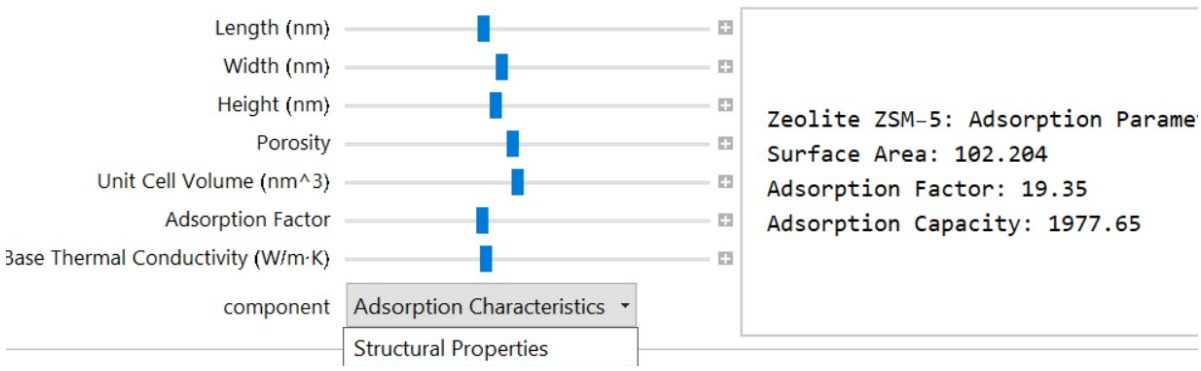
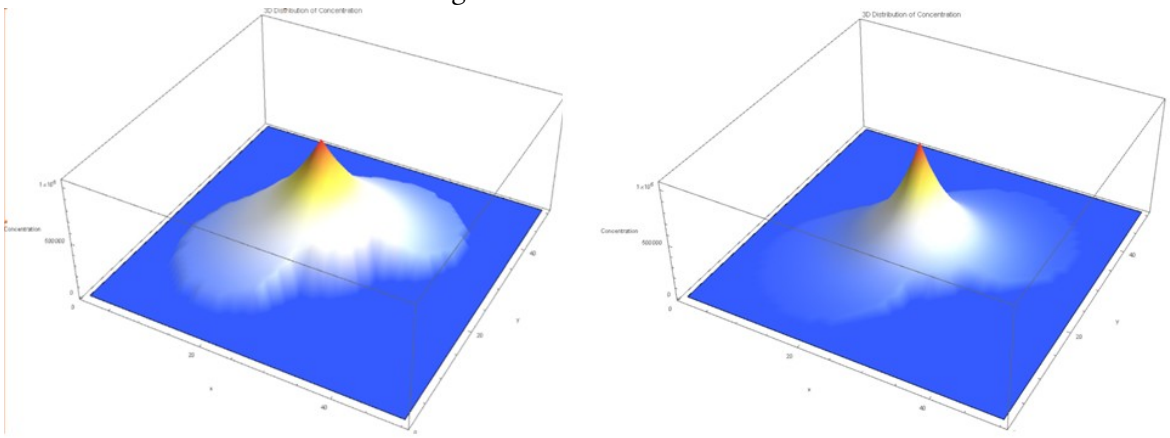


Figure 5: User interface when working with input parameters of the studied sample.

As seen from Figure 5, the user of the software system can effectively change the geometric parameters of the studied sample in the mathematical model, while the input physicochemical parameters can only be varied within realistic limits for a given material (in this case, ZSM-5 zeolite). After selecting the input parameters, the user can select from a drop-down menu one of the three components of the software system responsible for modeling the structural properties of the sample, its sorption characteristics, and thermal conductivity, respectively.

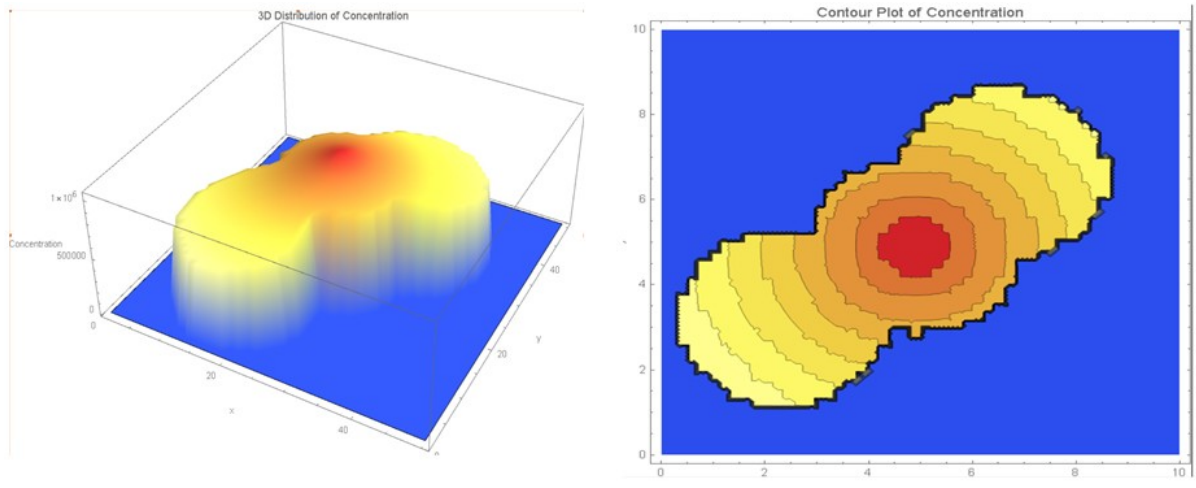
5. Testing the software system operation. Analysis of diffusion in various types of samples, visualization of results

At the first stage of verification of the developed mathematical models, a comparison was made of the results given by the analytical model (9) [9] with the results obtained on the basis of the finite-difference scheme implementation. For the calculations, a microstructure of a spherical sample with linear dimensions of 50 μm, based on ZSM-12 zeolite with a porosity of 0.3, and pore sizes of 50 nm was selected. Methane at a temperature of 300K was chosen as the diffused agent. The results of applying the software system components based on analytical and discretized mathematical models are shown in Figure 6.



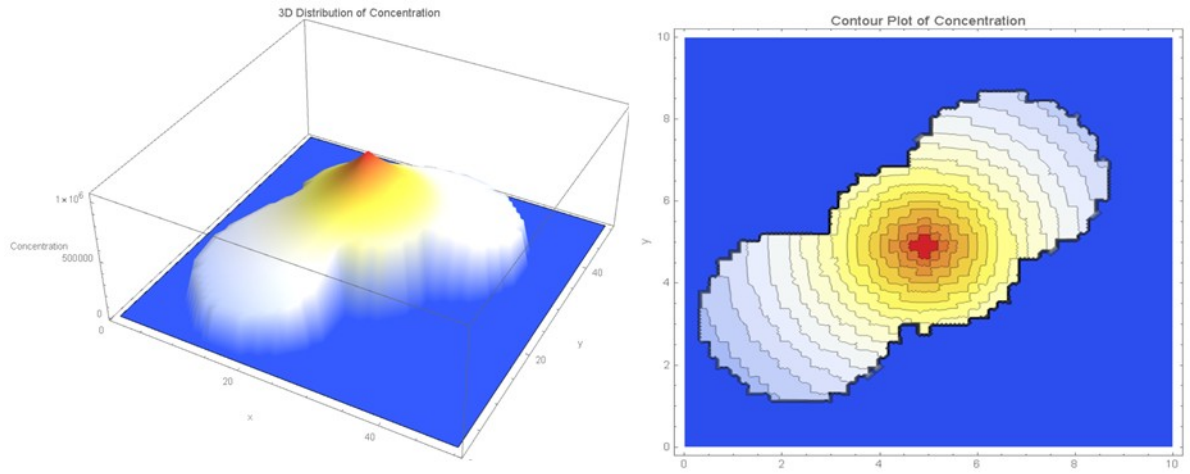
(a) (b)

Figure 6: Concentration distributions in a single-layer ZSM-12 zeolite in an analytical (a) and grid model (b).



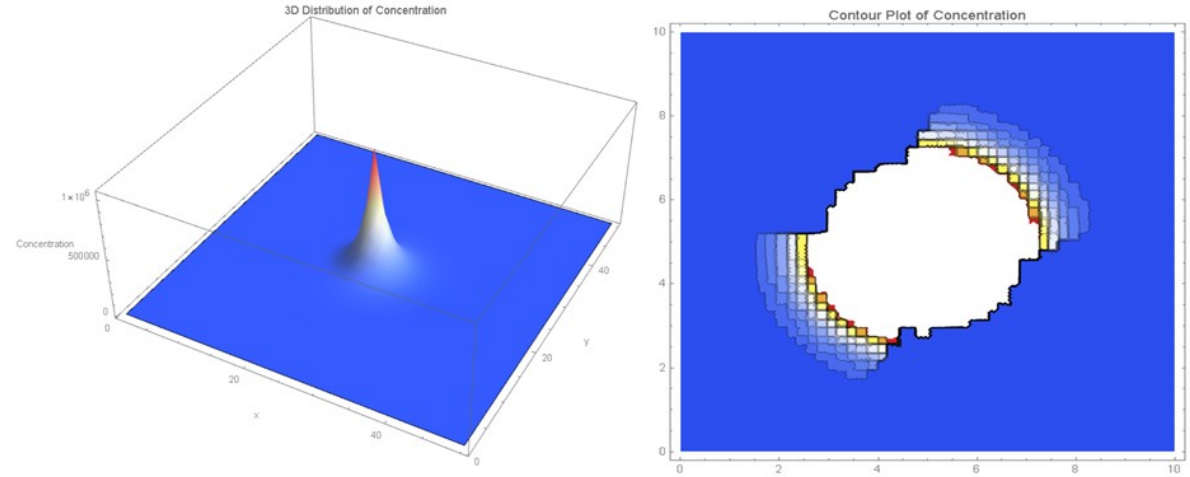
(a) (b)

Figure 7: Concentration distributions of ZSM-5 zeolite with 8 layers: spatial dependence (a) and cross-section (b).



(a) (b)

Figure 8: Concentration distributions of ZSM-12 zeolite with 20 layers: spatial dependence (a) and cross-section (b).



(a) (b)

Figure 9: Concentration distributions of ZSM-12 zeolite with 20 layers: spatial dependence (a) and cross-section (b).

The results of implementing both mathematical models give a similar and close result, which indicates the reliability of these methods in application to single-layer samples. Further, using the developed software for finite difference schemes, mathematical modeling of spatial distributions and their cross-sections was performed for various types of samples made of different materials, but their number of layers corresponds to experimentally realized configurations. Figure 7 shows the results of such calculations for a sample with 8 layers of ZSM-5 zeolite with porosity from 0.1 to 0.45.

Materials based on ZSM-12 zeolite usually have a large number of layers, the results calculated for a sample with 20 layers are shown in Figure 8. From the calculated dependencies, it is clearly seen that ZSM-11 zeolite has a much higher adsorption capacity than ZSM-5 zeolite, in particular due to a more uniform filling of pores in each of the sample layers.

Finally, we applied the software package to a sample made of a common and frequently used material – silica gel. The calculated dependencies are shown in Figure 9. As can be seen, the silica gel sample strongly loses in adsorption properties to all samples made on the basis of zeolites. The maximum concentration of the absorbed agent is obtained in the centre of the sample, and a significant part of it does not participate in the absorption process.

6. Conclusions

Mathematical models describing diffusion processes in material samples with nanoscale and microscale pores – have been constructed. A comparison of the developed mathematical models has been performed for their suitability to describe physicochemical processes in real technological conditions.

For the developed mathematical models, their discretization has been performed by applying the finite difference method to the equations describing diffusion transfer processes and boundary conditions that define the transfer balance in real existing material samples; Based on the obtained discretized mathematical models, their representation as grid problems has been performed. For each grid problem, the algorithmization of their solution by direct and reverse sweep methods in the Wolfram Mathematica environment has been carried out.

The architecture of the software system has been developed, which consists of software blocks implementing the grid problems of the diffusion mathematical models we have considered. The software system also contains a developed user interface that allows convenient variation of the parameters of mathematical models, geometric dimensions and physicochemical parameters of the studied samples.

The verification of the developed mathematical models and the software implementing them has been performed using experimentally realized samples and by testing the components of the software system for performance and realism of the obtained results.

In summary, it can be concluded that the developed software system and the components implemented in it will be directly useful both for researchers working in the field of heat and mass transfer modeling and for specialists engaged in solving specific technological problems. They can easily use the developed software product to quickly obtain the necessary active parameters for the mathematical models of the studied samples.

Declaration on Generative AI

The authors have not employed any Generative AI tools.

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