A Model of the Degrading Solute Transport in Porous Media based on the Multi-Stage Kinetic Equation

Bakhtiyor Khuzhayorov
Samarkand State University, Samarkand, Uzbekistan
b.khuzhayorov@mail.ru

Bekzodjon Fayziev
Samarkand State University, Samarkand, Uzbekistan
fayzievbm@mail.ru (corresponding author)

Otabek Sagdullaev
Kattakurgan Branch of Samarkand State University, Samarkand, Uzbekistan
otabek892603@gmail.com

Jamol Makhmudov
Samarkand State University, Samarkand, Uzbekistan
j.makhmudov@inbox.ru

Usmonali Saydullaev
Samarkand State University, Samarkand, Uzbekistan
sayus1979@mail.ru

Received: 13 September 2024 | Revised: 8 December 2024 | Accepted: 18 December 2024

ABSTRACT

A mathematical model of solute transport in porous media with two adsorption zones was developed, incorporating balance and kinetic equations, and initial and boundary conditions. The model was enhanced to account for multistage deposition kinetics in both adsorption zones, and numerical methods were employed to solve the problem. An algorithm using the finite difference method was presented as a solution. Computer experiments were conducted to ascertain the effect of different parameters of the model on solute transport, and the results of the study were analyzed. The primary focus of this study is to assess the impact of parameters within the kinetic equations on the transport process. These parameters are crucial in determining the intensity of adsorption during various stages of the process. The findings of this study demonstrate that multistage deposition kinetics significantly influences both the transport and adsorption processes. Furthermore, the presence of two distinct intensity areas in the concentration profile of the adsorbed substance is observed. This phenomenon is attributed to the effects of multistage kinetics.

Keywords-degradable solution; finite differences; mathematical model; porous medium; solute transport

I. INTRODUCTION

Degradable solute transport in porous media is a phenomenon that plays a significant role in various ecological [1], geological [2], and manufacturing [3] processes. Porous media can be found in natural and engineered systems, including soils, aquifers, oil reservoirs, and chemical reactors, among many others [4]. A comprehensive understanding of solute transport and transformation in these porous structures is imperative for addressing a wide range of challenges, including groundwater contamination, soil remediation, oil recovery, and the design of filtration systems [5]. One of the most widely employed methods for analyzing these problems is through modeling and simulation [6]. A significant aspect of solute transport in porous media is the degradation of pollutants [7, 8]. Degradation can be defined as the chemical or biological changes that occur during the process of solute transport in porous media. These processes are frequently observed under conditions conducive to the degradation of pollutants, involving pesticides [9], heavy metals, and organic matter [10, 11], through a variety of mechanisms, including chemical reactions, microbial activity, and abiotic processes. The ability to predict and control solute transport and degradation is imperative to ensure the safety and sustainability of water resources, reduce environmental pollution, and optimize industrial processes. The modeling of solute transport in a porous medium typically involves the use of convective-diffusion equations [8]. However, these models are further complicated by the consideration of solute interactions with the solid matrix, including chemical reactions that lead to adsorption, desorption, and degradation. The intricate interplay among these processes renders the study of solute transport in porous media a multifaceted endeavor, necessitating a comprehensive and nuanced approach to analysis. A plethora of models have been developed to describe the migration and degradation of solutes in porous media [7-11], ranging from simple analytical methods to complex numerical methods [12]. These models generally entail the resolution of partial differential equations, which encompass convection, diffusion, dispersion, and reaction kinetics. The selection of a model is contingent upon the particular characteristics of the system under investigation, encompassing the properties of the pore medium, the nature of the solute, and the flow conditions. Despite the advances in solute transport modeling, significant challenges persist in accurately predicting solute transport in porous media under complex conditions, where the changes in the pore structure, flow rates, and reaction rates are complex and non-linear. The intricate interplay among numerous concurrent processes and properties contributes to the complexity of solute transport. Among the nonequilibrium processes influencing transport are degradation and adsorption. Adsorption, defined as the adhesion of solutes to the surface of a solid skeleton (walls) of a porous medium, influences the migration and distribution of solutes over time. The formulation of kinetic equations that govern adsorption processes is imperative for accurate modeling and prediction of solute transport in porous media. The reversibility or irreversibility of adsorption is determined by the nature of interactions between the solute and the solid surface [8]. In the context of degraded solutions, adsorption can either enhance or inhibit the degradation process.

Kinetic equations are a critical component of the scientific study of adsorption, as they provide a quantitative framework for understanding the dynamics of solute migration processes [13]. These equations are critical for comprehending the interactions of solutes with porous media and for predicting their behavior in natural and engineered systems. The incorporation of adsorption kinetics into transport models facilitates a more precise modeling of the temporal and spatial distribution of solutes. The nature of the adsorption process and the interaction between the solute and the solid surface are the two main factors that determine the classification of adsorption kinetics [14]. The most common kinetic models include the following:

- Linear adsorption (first-order kinetics): In this model, the rate of adsorption is directly proportional to the solute concentration in the liquid phase.
- Langmuir adsorption kinetics: The Langmuir model predicts that adsorption occurs at a limited number of uniform sites on a solid surface without interactions between the adsorbed molecules [15].
- Freundlich adsorption kinetics: The Freundlich model is an empirical model describing adsorption on heterogeneous surfaces whose adsorption capacity varies with solute concentration [16].

The adsorption process bears similarity to the deposition of suspended particles in porous media [17]. In recent years, multi-stage kinetics has been widely used to represent the deposition kinetics of suspended particles [18-20]. This paper employs the multistage kinetics equation for the adsorption process for the first time. This approach enables the consideration of phenomena occurring during the adsorption process that are not fully captured by a one-stage kinetic equation. The resolution of problems pertaining to solute transport in a porous medium typically entails the usage of three primary methodological approaches: Firstly, analytical methods are employed, followed by numerical methods, and finally, semi-analytical methods [12]. Analytical methods provide exact solutions to the governing transport equations under specific initial and boundary conditions. These solutions are expressed in closed mathematical forms, offering precise insights, but are often limited to simplified scenarios. Numerical models, on the other hand, rely on computational methods, such as finite difference or finite element techniques, to approximate solutions. These models are particularly well-suited for complex systems, where analytical solutions are impractical due to irregular geometries or heterogeneous conditions. Semi-analytical models are a synthesis of the two approaches, combining the precision of analytical methods with the flexibility of numerical approaches. These models employ a combination of closed-form solutions and numerical methods to solve transport equations, thereby offering enhanced flexibility while maintaining a degree of analytical rigor. Due to the inherent complexity of the problem, numerical methods are employed in this study. The objective of this paper is to enhance the comprehension of solute transport processes in porous media by incorporating considerations of solute degradation and multistage adsorption kinetics. The study examines the main factors affecting solute transport and degradation, including the physical properties of the pore medium, the chemical nature of the solute, and environmental conditions. The development and application of mathematical models are central to the paper's objective of elucidating the mechanisms underlying solute adsorption and degradation. The models developed and employed in this study are designed to provide insights into these mechanisms and to suggest strategies that could enhance the prediction and control of solute migration in porous media. The study focuses on the simultaneous adsorption and degradation of a solute taken pesticide. Degradation is defined as the process by which a compound is broken down into simpler components, such as water, carbon dioxide, and ammonia, through chemical reactions, like hydrolysis, photolysis, and biodegradation [8]. To address this challenge, a numerical algorithm has been developed based on a finite difference scheme. The reliability and stability of the method are thoroughly examined. The model was reduced to a one-dimensional case by leveraging the symmetry properties of the porous media. The numerical algorithm developed in this paper can be readily employed for 2D and 3D cases by using the alternating direction method, which involves the separate determination of function values in each coordinate direction for a new time layer. The numerical solution of the problem has been used to estimate the role of the multistage characteristics of adsorption on solute transport. The objective of this study is to enhance the comprehension of solute transport, adsorption, and degradation in porous media, thereby establishing a foundation for future research and practical applications in environmental engineering, hydrogeology, and associated domains.

II. PROBLEM STATEMENT AND MATHEMATICAL MODEL

Figure 1 shows a schematic representation of the process of filling the pore volume. This study examines a two-zone porous medium comprising active and passive zones. The migration equation, incorporating the processes of adsorption and decay, can be expressed as [8]:

$$\frac{\partial(\theta c)}{\partial t} = -divJ - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda c \tag{1}$$

$$J = -\theta D \nabla c + \vec{w} c \tag{2}$$

where c is the volumetric concentration, c_a is the concentration of the adsorbed substance in the active zone, c_p is the concentration of the adsorbed substance in the passive zone, J is the flow density of the solute, θ is the porosity, λ is the first-order decay coefficient (degradition), $\vec{w}$ is the velocity, $\frac{\partial c_a}{\partial t}, \frac{\partial c_p}{\partial t}$ are the terms of adsorption in the active and passive zones, respectively, and refer to the mass transfer between the liquid phase and the solid surface due to adsorption phenomena. Substituting (2) into (1):

$$\frac{\partial(\theta c)}{\partial t} + div(\vec{w} c) = div(\theta D \nabla c) - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda c \tag{3}$$

From (3), we have the following in one-dimensional case:

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial}{\partial x}(w_x c) = \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda c \tag{4}$$

where w_x is the coordinate of the velocity along the Ox axis. In the event that the medium is homogeneous, that is, θ = const, it can be demonstrated that the filtration rate and the hydrodynamic dispersion coefficient in (4) are constant as well:

$$\frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - \frac{1}{\theta}\frac{\partial c_a}{\partial t} - \frac{1}{\theta}\frac{\partial c_p}{\partial t} - \lambda c \tag{5}$$

where $v_x = \frac{w_x}{\theta}$ is the physical velocity of the fluid. The following kinetic equation is employed to ascertain the concentration of the adsorbed substance in the active zone [17]:

$$\frac{\partial c_a}{\partial t} = \beta_a \left(c - \frac{c_a}{c_{a0}} c_0\right) - \lambda_a c_a \tag{6}$$

where β_a is the coefficient describing the adsorption intensity of the substance in the active zone, c_{a0} is the maximum concentration of adsorbed substance that can be achieved in the active zone, and λ_a is the decay coefficient of the adsorbed substance in the liquid zone. In this instance, rather than employing (6), it is more appropriate to use the following multistage kinetics [20]:

$$\frac{\partial c_a}{\partial t} = \begin{cases} \beta_{ar} c - \lambda_a c_a, 0 < c_a \le c_{ar}, \\ \beta_{aa} c - \beta_{ad} c_a - \lambda_a c_a, 0 < c_a < c_{ar}, \\ 0, c_a = c_{a0}, \end{cases} \tag{7}$$

where $\beta_{ar}, \beta_{aa}, \beta_{ad}$ are kinetic coefficients, c_{ar} is the maximum concentration at which the “charging” effect ends.

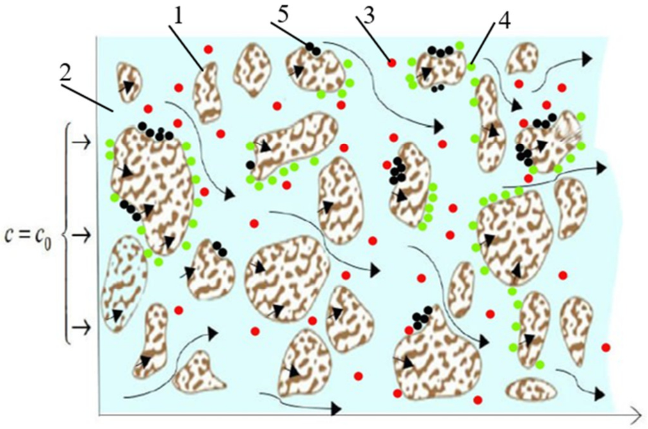

Fig. 1. Schematic of filling the pore volume: (1) grains of the skeleton of the medium, (2) carrier phase of the solute, (3) mobile particles of the solute, (4) adsorbed particles of the solute in active zone, (5) adsorbed particles of the solute in passive zone.

Equation (6) is modified for the active zones of the filter on the basis of the following physical idea [20]: initially, adsorption occurs in the porous media that is free of solute particles. During the initial accumulation of solute particles, the specific surface area increases, and consequently, the kinetic coefficients also increase. This phenomenon, known as filter charging, exerts a substantial influence during the nascent stages of adsorption [17]. This process persists until the surface of the grains in the medium is covered with a monolayer of solute particles. Subsequent to this, the particles commence interaction with a previously adsorbed layer, thereby progressing to the subsequent stage of the adsorption cycle, characterized by particle retention. The processes of solute particle adsorption and their release by liquid flow occur in parallel [18]. The transition of adsorption from the irreversible to reversible stages is marked by the attainment of a specific adsorption concentration, c_{ar}, which is a critical value in this process. At the final stage, the adsorption of solute particles reaches a maximum possible value c_{a0}, which is defined as the point at which the active zone of the porous medium is fully saturated with solute particles. At this stage, the concentration of the adsorbed solute particles remains constant over time. The kinetic equation of adsorption in the passive zone is [16]:

$$\frac{\partial c_p}{\partial t} = \beta_p(c_p)c - \lambda_p c_p \tag{8}$$

where λ_p is coefficient of decay of the adsorbed substance in the passive zone, $\beta_p = \alpha(c_p)\beta_{p0}$.

$$\alpha(c_p) = \begin{cases} 1, c_p \le c_{p1}, \\ \frac{c_{p1}}{c_p}, c_{p1} < c_p < c_{p0}, \\ 0, c_p = c_{p0}, \end{cases} \quad (9)$$

where c_{p1} is the concentration at which the aging effect begins. Considering (9), we rewrite (8) as:

$$\frac{\partial c_p}{\partial t} = \begin{cases} \beta_{p0} c - \lambda_p c_p, 0 < c_p \le c_{p1} \\ \beta_{p0} \frac{c_{p1}}{c_p} c - \lambda_p c_p, c_{p1} < c_p < c_{p0} \\ 0, c_p = c_{p0}. \end{cases} \quad (10)$$

Equations (5), (7), and (10) are solved with the following initial and boundary conditions:

$$c(0,x) = 0, c_a(0,x) = 0, c_p(0,x) = 0 \quad (11)$$

$$c(t,0) = c_0 = const, c(t,\infty) = 0 \quad (12)$$

III. SOLUTION ALGORITHM

The finite difference method is deployed to solve (5), (7), and (10) to (12) [21]. In the area $D = \{0 \le x < \infty,\ 0 \le t \le T\}$ a grid $\omega_{h\tau}$ is introduced, where T is the value of time in which the process is under study. On the axis Ox the interval $0, \infty)$ is divided by step h and the time interval $[0, T]$ is divided by step τ. To approximate the equations, the following grid is introduced:

$$\omega_{h\tau} = \left\{ (x_i, t_j),\ x_i = ih, i = 0,1,\dots, t_j = j\tau,\ j = \overline{0,J}, \tau = \frac{T}{J} \right\}$$

Instead of the functions $c(t,x)$, $c_a(t,x)$, $c_p(t,x)$, specific functions are considered, whose values at the nodes (x_i, t_j) are defined as c_i^j, $c_{a,i}^j$, $c_{p,i}^j$, respectively. With (5) we approximate in the following form on the grid $\omega_{h\tau}$:

$$\frac{c_i^{j+1} - c_i^j}{\tau} + v_x \frac{c_i^{j+1} - c_{i-1}^{j+1}}{h} = D \frac{c_{i+1}^{j+1} - 2c_i^{j+1} + c_{i-1}^{j+1}}{h^2} - - \frac{1}{\theta} \frac{c_{a,i}^{j+1} - c_{a,i}^j}{\tau} - \frac{1}{\theta} \frac{c_{p,i}^{j+1} - c_{p,i}^j}{\tau} - \lambda c_i^{j+1} \quad (13)$$

The differential schemes for (7) and (10) are:

$$\frac{c_{a,i}^{j+1} - c_{a,i}^j}{\tau} = \begin{cases} \beta_{ar} \nu c_i^j - \lambda_a c_{a,i}^j, 0 < c_{a,i}^j \le c_{ar}, \\ \beta_{aa} \nu c_i^j - \beta_{ad} c_{a,i}^j - \lambda_a c_{a,i}^j, c_{ar} < c_{a,i}^j < c_{a0}, \\ 0, c_{a,i}^j = c_{a0}. \end{cases} \quad (14)$$

$$\frac{c_{p,i}^{j+1} - c_{p,i}^j}{\tau} = \begin{cases} \beta_{p0} c_i^j - \lambda_p c_{p,i}^j, 0 < c_{p,i}^j \le c_{p1}, \\ \frac{\beta_{p0} c_{p1} c_i^j}{c_{p,i}^j} - \lambda_p c_{p,i}^j c_{p1} < c_{p,i}^j < c_{p0}, \\ 0, c_{p,i}^j = c_{p0}. \end{cases} \quad (15)$$

The initial and boundary conditions (11), (12) have the form:

$$c_{a,i}^j = 0, i = \overline{0,I}, j = 0, c_{p,i}^j = 0, i = \overline{0,I}, j = 0, c_i^j = 0, i = \overline{0,I}, j = 0, c_i^j = 0, i = 0, j = \overline{0,J} \quad (16)$$

where *I* is sufficiently large value, for which $c_I^j = 0$ is true. First, by using the initial conditions, c_i^j, $c_{a,i}^j$, $c_{p,i}^j$ are found in the zero-time layer. Then, (15) is used to find $c_{p,i}^{j+1}$ and (14) for $c_{a,i}^{j+1}$. Finally, substituting $c_{a,i}^j$ and $c_{p,i}^j$ into (13), by using Thomas' algorithm, we determine c_i^j on the *(j+1)* th layer of the grid $\omega_{h\tau}$.

IV. RESULTS AND DISCUSSION

A numerical experiment was conducted using a computer program developed by the authors in Python. A thorough examination of the numerical outcomes is warranted. As shown in Figure 2, three concentration fields (*c*/*c*₀, *c*ₐ, *c*ₚ) are presented, demonstrating a gradual penetration of all three concentrations into the inner side of the porous medium over time.

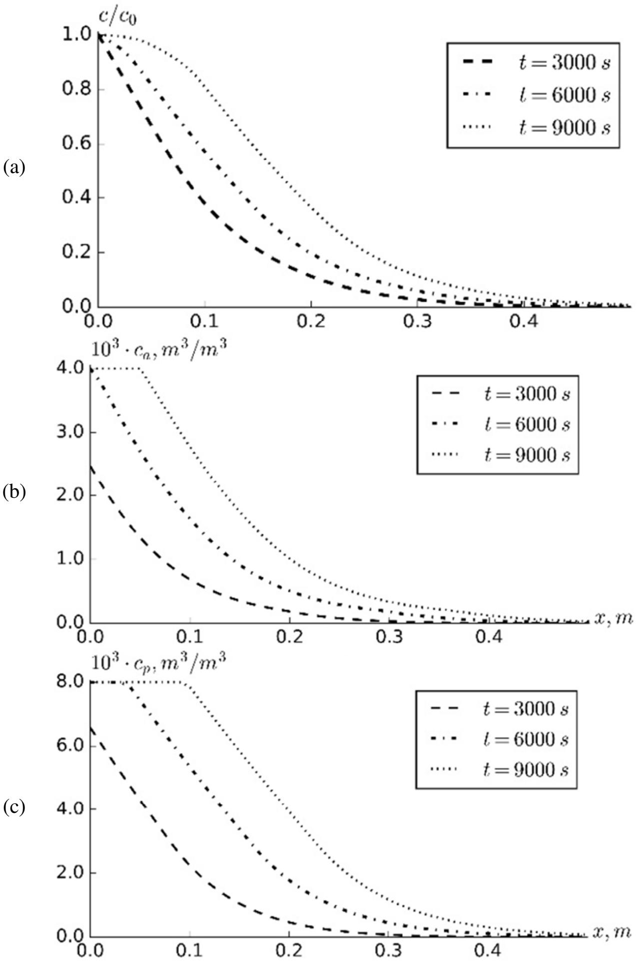

Fig. 2. Profiles of changes: (a) c/c_0, (b) c_a, (c) c_p, at $c_{p1} = 3 \times 10^{-3}$m³/m³ and various time values.

Specifically, at *t*=3000 s, the substance concentration has attained the projected distance of 0.37 m. At *t*=6000 s, it surpasses 0.4 m, and at *t*=9000 s, it approaches a concentration of 0.5m. At *t*=3000 s, it is evident that both concentrations, c_a and c_p, have not yet attained their saturation value. In this instance, the adsorbed substance in the active zone was approximately 65% of its maximum value, while in the passive zone, this indicator was around 80%. Subsequently, at *t*=6000 s, it was observed that the adsorbed substance attained its maximum value in both zones.

At this time, the saturation in the passive zone is more widespread than in the active zone of the parameter β_aa, which is the attachment coefficient, indicating the rate of adsorption in the expression that represents the primary step of the equation of the kinetics of substance adsorption in the active zone. It can be observed that the change in its value has a significant effect on the rate of substance adsorption in the active zone, as illustrated in Figure 3.

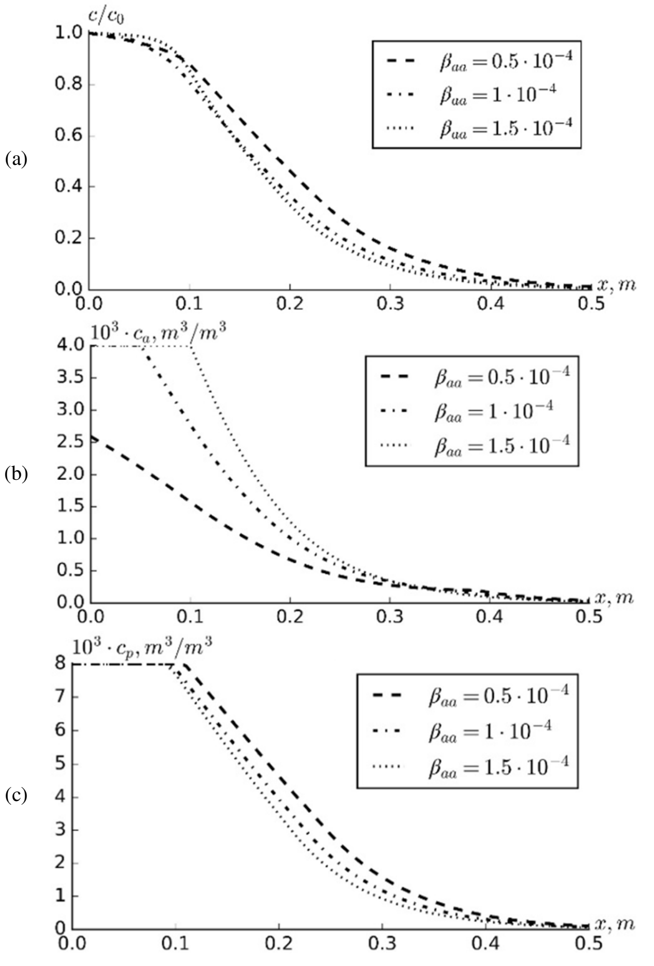

Fig. 3. Profile of: (a) c/c_0, (b) c_a, (c) c_p, at $t = 9000$ s and different values of β_{aa}.

It can be noted that the substance adsorbed in the active zone has not reached its maximum value at the point $x = 0$ when reduced to $\beta_{aa} = 0{,}5 \cdot 10^{-4}$ at $t = 900$ s. However, this indicator reached its maximum value when $\beta_{aa} = 1 \cdot 10^{-4}$ or $\beta_{aa} = 1{,}5 \cdot 10^{-4}$. Smaller values of β_{aa} led to a decrease in $c_a$and an increase and wider spread of c/c_0, c_p at fixed points. Figure 4 facilitates the study of the effect of the parameter β_{ad}, which evaluates the intensity of substance desorption process during the main phase of substance adsorption in the active zone. As demonstrated in Figure 4 (b), an increase in β_{ad} results in a substantial decrease in the adsorbed substance concentration, c_a, within the active zone. This, in turn, leads to an increase in c_p, as displayed in Figure 4 (c). It is possible to estimate the effect of β_{ad} on the profiles of c/c_0. It is evident that an augmentation in β_{ad} results in a decline of c/c_0, particularly at points in proximity to *x*=0 and at points that are distant from *x*=0. Conversely, an increase in β_{ad} leads to an increase of c/c_0. This phenomenon can be attributed to the observation that, with an increase in β_{ad}, the attainment of maximum value of c_a, corresponding to the state of dynamic equilibrium, is hindered. Consequently, the achievement of the maximum value of c/c_0 is postponed. Figure 5 depicts the impact of the parameter β_{ar} on the process, which is the coefficient representing the intensity of substance adsorption in the active zone during the loading stage, and since it lasts for a short time, it can be observed that the effect of β_{ar} is not too great. The effect of β_{ar} is primarily discernible in the concentration of the adsorbed substance, c_a, within the active zone.

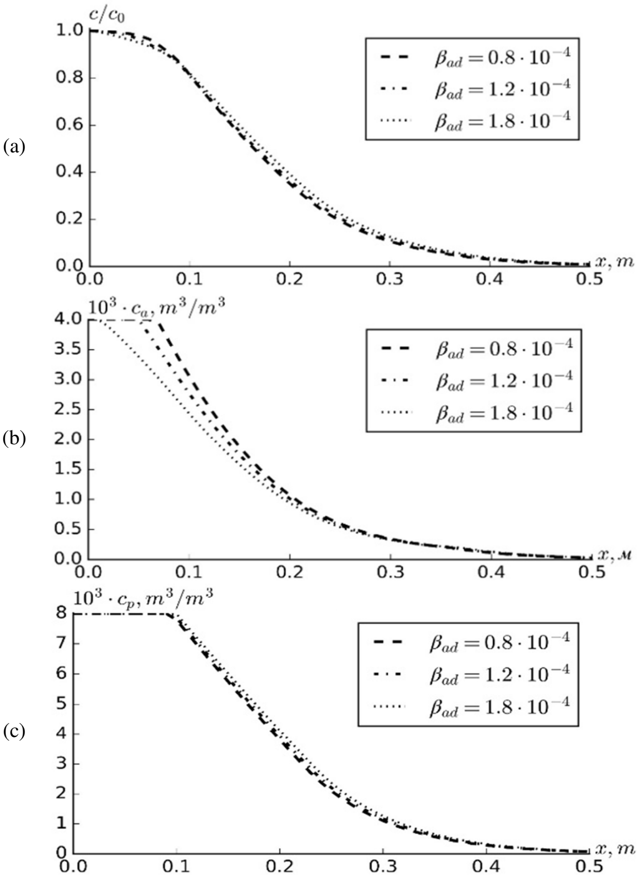

Fig. 4. Profile of (a) c/c_0, (b) c_a, (c) c_p, at $t = 9000$ s and different values of β_{ad}.

As evidenced by the graphs, increasing the value of β_{ar} results in an increase in the concentration c_a, along with a negligible decrease in c_p. Furthermore, an increase in β_{ar} leads to a decrease in the concentration c/c_0, despite the minimal change in the value of c_p. As shown in Figure 6, the dynamics of concentrations c/c_0, c_a, c_p are observed at three fixed points within the environment. The dynamics of relative concentration (c/c_0) exhibited a substantial increase in the initial values of time at all three points. Subsequently, the rate of increase decreased significantly.

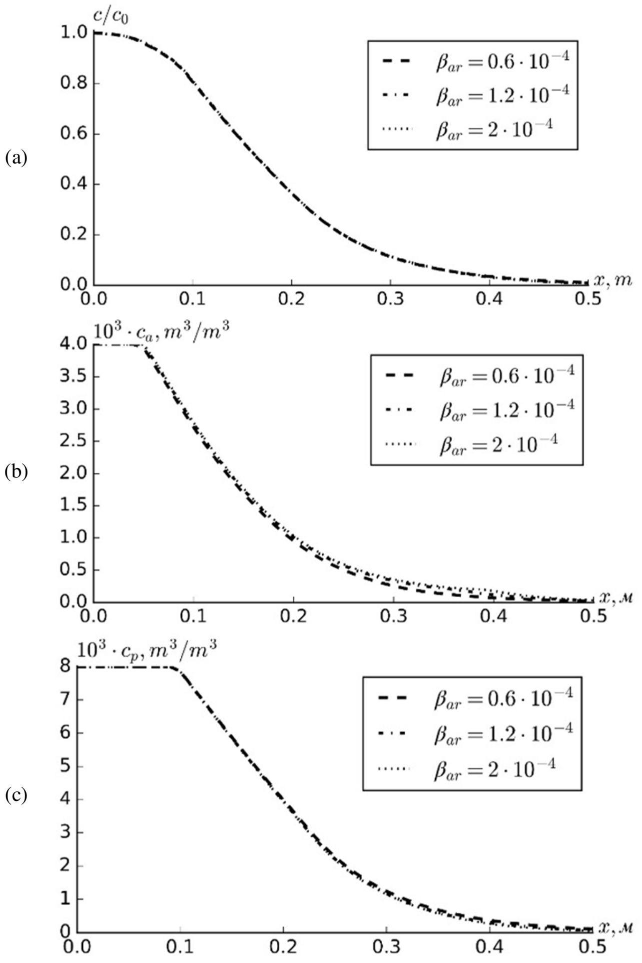

Fig. 5. Profile of: (*a*) c/c_0, (*b*) c_a, (c) c_p, at $t = 9000$ s and different values of β_{ar}.

In order to comprehend the circumstances under consideration, a detailed examination of Figures 6 (b) and 6 (c) is imperative. The adsorption process in both zones was considered on the basis of multi-stage kinetic equations. It was determined that the intensity of adsorption is directly proportional to the concentration of the substance in the medium. Therefore, adsorption occurs more slowly at smaller values of time. It is also noteworthy that the intensity of adsorption in the initial loading phase in the active zone is significantly lower than in the main phase. During the designated interval, the concentration of the adsorbed substance attained its maximum value in the passive zone at approximately t = 4500 s and in the active zone at approximately t = 6500 s. The maximum value of c/c_0 was achieved with a slight delay, and at the point $x = 0.06$, only c_p reached its maximum value.

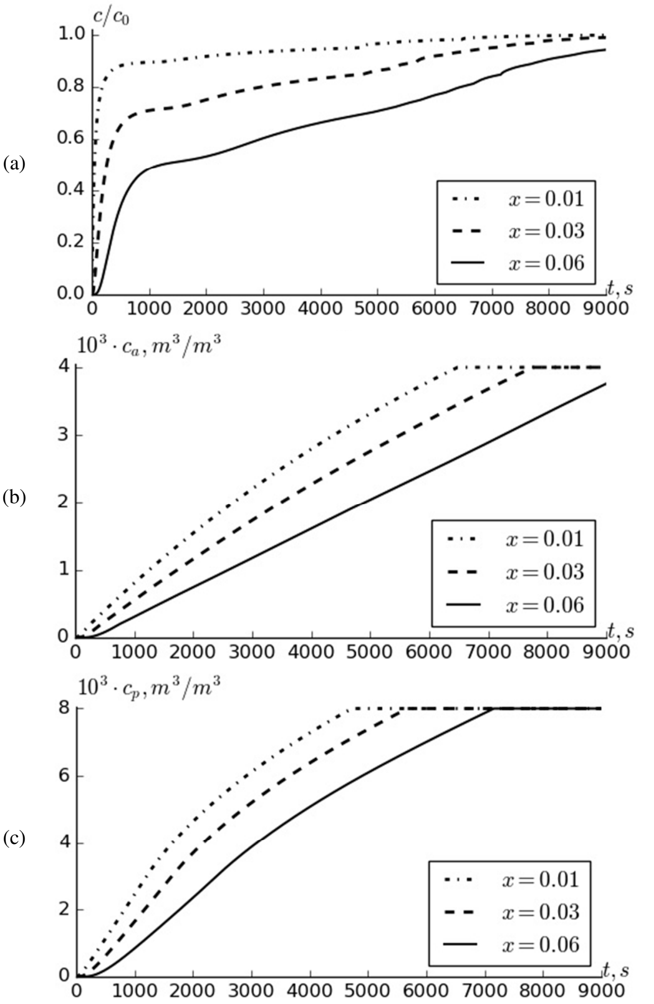

Fig. 6. Dynamics of change: (*a*) c/c_0, (*b*) c_a, (c) c_p, at different values of x.

As shown in Figure 7, the solutions for the case in which the value of c_{a1} is increased from 2×10^{-4} to 8×10^{-4} are demonstrated. It is evident that as the value of c_{a1} is increased, two distinct intensity areas emerge within the concentration profile of the adsorbed substance c_a. This phenomenon can be attributed to the multi-stage kinetics equation employed within the active zone. With a further increase in the value of c_{a1}, the distinction between these fields becomes more pronounced. Conversely, an increase in c_{a1} results in a decrease in the rate of substance adsorption within the passive zone.

V. CONCLUSIONS

This article examines the solute transport in porous media with varying types of adsorption zones. The solute is regarded as an active substance, and the processes of degradation and adsorption in the active and passive zones of the porous medium are taken into account. The solute transport problem for the one-dimensional case is numerically solved using the finite difference method. The concentration fields and the concentration of the adsorbed solute are determined for both the passive and active zones.

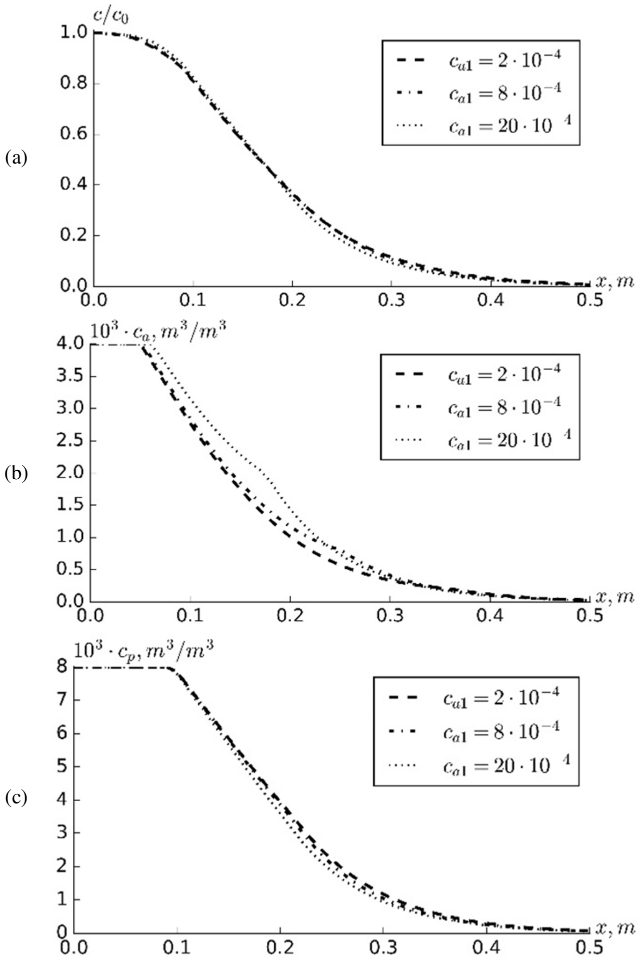

Fig. 7. Profiles of changes: (*a*) c/c_0, (*b*) c_a, (*c*) c_p, at $t = 9000$ s and various values $of\ c_{a1}$.

In this study, multistage kinetics equations for adsorption were examined for the first time. It has been demonstrated that the multistage dynamics of adsorption, which are characterized by the various features of each stage and their parameters, can result in a variety of effects that are not characteristic of solute transport with one-stage adsorption kinetics. Specifically, the presence of two distinct intensity areas in the concentration profile of the adsorbed substance in the active zone is evidenced and explained by the multi-stage kinetics equation employed in this zone. Furthermore, an increase in the attachment coefficient parameter has been observed to result in enhanced adsorption within the passive zone. Consequently, the acceleration of adsorption in the passive zone results in a modest decline in the concentrations of the solute transport and the adsorbed substance in the active zone. When the value of the charging parameter for the active zone is increased, the presence of two distinct intensity areas in the concentration profile of the adsorbed substance is observed, which is not characteristic of one-stage adsorption kinetics. The degradation coefficients in the transport equations are assumed to be equal in the case of a radioactive solute. The employment of multistage kinetics equations facilitates the consideration of all stages within the adsorption process. However, this approach renders the mathematical model considerably more complex, making analytical solution impossible.

NOMENCLATURE

J	Flow density of the solute
c	Volumetric concentration
c_a	Concentration of the adsorbed substance in the active zone
c_{a0}	Maximum concentration of adsorbed substance that can be achieved in the active zone
c_{ar}	Maximum concentration at which the charging effect ends
c_p	Concentration of the adsorbed substance in the passive zone
c_{p1}	Concentration at which the "aging" effect begins
v_x	Physical velocity of the fluid
$\vec{w}$	Velocity
w_x	Coordinate of the velocity along the Ox axis
β_a	Coefficient describing the adsorption intensity of the substance in the active zone
β_{aa}	Kinetic coefficients of attachment for main stage in active zone,
β_{ar}	Kinetic coefficient of attachment for “charging” stage in active zone
β_{ad}	Kinetic coefficients of detachment for main stage in active zone
β_p	Kinetic coefficients of attachment for main stage in passive zone,
λ	First-order decay coefficient (degradition)
λ_a	Decay coefficient of the adsorbed substance in the active zone
λ_p	Coefficient of decay of the adsorbed substance in the passive zone,
θ	Porosity
a	Active zone
p	Passive zone
ar	Charging stage for active zone
aa	Attachment coefficient for active zone
ad	Detachment coefficient for active zone
x	Ox axis
i	Grid nods for coordinate
j	Grid nods for time

REFERENCES

[1] L. Zeng *et al.*, "Research on the Migration and Adsorption Mechanism Applied to Microplastics in Porous Media: A Review," *Nanomaterials*, vol. 14, no. 12, Jan. 2024, Art. no. 1060, https://doi.org/10.3390/nano14121060.

[2] B. Berkowitz, I. Dror, S. K. Hansen, and H. Scher, "Measurements and models of reactive transport in geological media," *Reviews of Geophysics*, vol. 54, no. 4, pp. 930–986, 2016, https://doi.org/10.1002/2016RG000524.

[3] J. Bear and J.-M. Buchlin, Eds., "Modelling and Applications of Transport Phenomena in Porous Media," in *Theory and Applications of*

Transport in Porous Media, vol. 5, Dordrecht, Netherlands: Springer Netherlands, 1991.

[4] C. Tien and B. V. Ramarao, *Granular Filtration of Aerosols and Hydrosols*, 2nd ed. Boston, MA, USA: Butterworth-Heinemann, 1989.

[5] C. W. Fetter, T. Boving, and D. Kreamer, *Contaminant Hydrogeology*, 3rd ed. Long Grove, IL, USA: Waveland Press, 2017.

[6] M. Alquraish, "Modeling and Simulation of Manufacturing Processes and Systems: Overview of Tools, Challenges, and Future Opportunities," *Engineering, Technology & Applied Science Research*, vol. 12, no. 6, pp. 9779–9786, Dec. 2022, https://doi.org/10.48084/etasr.5376.

[7] A. V. Ogram, R. E. Jessup, L. T. Ou, and P. S. Rao, "Effects of sorption on biological degradation rates of (2,4-dichlorophenoxy) acetic acid in soils," *Applied and Environmental Microbiology*, vol. 49, no. 3, pp. 582–587, Mar. 1985, https://doi.org/10.1128/aem.49.3.582-587.1985.

[8] M. T. van Genuchten and R. J. Wagenet, "Two-Site/Two-Region Models for Pesticide Transport and Degradation: Theoretical Development and Analytical Solutions," *Soil Science Society of America Journal*, vol. 53, no. 5, pp. 1303–1310, 1989, https://doi.org/10.2136/sssaj1989.03615995005300050001x.

[9] J. R. Mover, R. J. Hance, and C. E. McKone, "The effect of adsorbents on the rate of degradation of herbicides incubated with soil," *Soil Biology and Biochemistry*, vol. 4, no. 3, pp. 307–311, Aug. 1972, https://doi.org/10.1016/0038-0717(72)90026-0.

[10] M. L. Brusseau, L. H. Xie, and L. Li, "Biodegradation during contaminant transport in porous media: 1. mathematical analysis of controlling factors," *Journal of Contaminant Hydrology*, vol. 37, no. 3, pp. 269–293, Apr. 1999, https://doi.org/10.1016/S0169-7722(99)00005-4.

[11] S. A. Kammouri, M. El Hatri, and J. M. Crolet, "Modeling Contaminant Transport and Biodegradation in a Saturated Porous Media," in *Computational Methods for Flow and Transport in Porous Media*, J. M. Crolet, Ed. Dordrecht Netherlands: Springer Netherlands, 2000, pp. 237–243.

[12] A. R. Estabragh, M. R. S. Pereshkafti, and A. A. Javadi, "Comparison Between Analytical and Numerical Methods in Evaluating the Pollution Transport in Porous Media," *Geotechnical and Geological Engineering*, vol. 31, no. 1, pp. 93–101, Feb. 2013, https://doi.org/10.1007/s10706-012-9566-6.

[13] A. K. Surela, L. K. Chhachhia, V. K. Surela, and P. L. Meena, "Polypyrrole-Based Composites for Dyes Removal From Contaminated Water," in *Reference Module in Materials Science and Materials Engineering*, Elsevier, 2024.

[14] M. H. El-Naas and M. A. Alhaija, "Modelling of adsorption processes," in *Mathematical Modelling*, New York, NY, USA: Nova Science Publishers, Inc., 2013, pp. 579–600.

[15] I. Langmuir, "The adsorption of gases on plane surface of glass, mica and platinum," *Journal of the American Chemical Society*, vol. 40, no. 9, pp. 1361–1403, Sep. 1918, https://doi.org/10.1021/ja02242a004.

[16] H. M. F. Freundlich, "Over the adsorption in solution," *The Journal of Physical Chemistry*, vol. 57, pp. 385–470, 1906.

[17] V. Venitsianov and R. N. Rubinstein, *Dynamics of Sorption from Liquid Media*. Moscow, Russia: Nauka, 1983.

[18] V. Gitis, I. Rubinstein, M. Livshits, and G. Ziskind, "Deep-bed filtration model with multistage deposition kinetics," *Chemical Engineering Journal*, vol. 163, no. 1, pp. 78–85, Sep. 2010, https://doi.org/10.1016/j.cej.2010.07.044.

[19] B. Fayziev, G. Ibragimov, B. Khuzhayorov, and I. A. Alias, "Numerical Study of Suspension Filtration Model in Porous Medium with Modified Deposition Kinetics," *Symmetry*, vol. 12, no. 5, May 2020, Art. no. 696, https://doi.org/10.3390/sym12050696.

[20] B. Kh. Khuzhayorov, J. M. Makhmudov, B. M. Fayziev, and T. I. Begmatov, "Some Model of a Suspension Filtration in a Porous Media ThatAccounts for the Two-Zone and Multistage Character of Deposition Kinetics," *Journal of Applied and Industrial Mathematics*, vol. 14, no. 3, pp. 513–523, Aug. 2020, https://doi.org/10.1134/S1990478920030102.

[21] A. A. Samarskii, *The Theory of Difference Schemes*, 1st ed. New York, NY, USA: CRC Press, 2001.