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EFFECT OF THE POLYMER NETWORK ON THE DIFFUSION OF FOREIGN PARTICLES IN HYDROGELS

In the present work, we introduce a physical model of foreign particle diffusion in polymer hydrogels that accounts for the network architecture of these systems. The model employs a classical diffusion theory framework in condensed media to derive a theoretical dependence of the diffusion coefficient on the volume occupied by the hydrogel's network. We demonstrate that the changes in the diffusion of foreign particles can be attributed to the changes in the free activation energy due to the presence of the polymer network. Using optical image analysis, we obtained the dependence of the diffusion coefficient in agarose and gelatine hydrogels on the concentration of the gelling agent. The experimental data obtained are in good agreement with the theoretical dependences predicted by the proposed physical model. Furthermore, when the size of the diffusing particles is much smaller than the hydrogel pore size, the diffusion coefficient appears to be independent of the nature of the hydrogel and determined solely by the gelling agent concentration.

K e y w o r d s : diffusion, hydrogels, agarose, gelatine, rhodamine, polymer network.

PACS classification: 66.30.-h, 82.70.Gg.

Introduction

A polymer hydrogel is a water-polymer system in which polymer chains form a network (Yuan et al., 2025; Zhu et al., 2023; Alekseev et al., 2019). These hydrogels are widely used in the pharmaceutical industry (Clegg et al., 2024; Yang, 2022; Mehta et al., 2023; Ho et al., 2022) for drug delivery systems. When a hydrogel 'loaded' with an active pharmaceutical ingredient is brought into contact with tissue, the diffusion flow of the API molecules is formed (Richtering et al., 2016). The rate of this flow is given by the diffusion equation (Birkhoff, 2015):

$$\boldsymbol{J} = -D\boldsymbol{\nabla}c, \tag{1}$$

where c is the concentration of API, and D is a diffusion coefficient.

This implies that the duration of drug action is, in part, determined by the rate of diffusion. Engineering the rate of diffusion thus offers an opportunity to modify a drug's half-life, as described, for instance, in (Smeets, & Hoare, 2013; Wang et al., 2020; Armstrong et al., 2014; Velasco et al., 2011), where the authors' work is empirical and practical. The knowledge gap, however, exists in the absence of a physical model of the diffusive motion of particles of enriching agents in hydrogels. The

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difference in the diffusion of such particles in hydrogels, compared to water, is primarily due to the network architecture (Roca-Arroyo et al., 2025; Zhu et al., 2025). Thus, in this work, we present the model of diffusion of foreign particles that accounts for the presence of a polymer network.

1. Theoretical model

1.1. Diffusion mechanism in condensed matter: general characteristics

The current understanding of the diffusion mechanism in condensed matter is based on the classical theory described in (Frenkel, 1955). This theory can be summarized as follows.

The particle that undergoes diffusion has position vectors given by $r_1, r_2, \dots, r_n$ at instances $t_1, t_2, \dots, t_n$. Each of the positions of the particle corresponds to a certain locally equilibrium state of the system, which contains this particle (Hnatiuk et al., 2023; Lazarenko et al., 2024; 2025). Let's denote the free energy of each of these states as $F_1, F_2, \dots, F_n$. The volumes in which the local equilibria are established, and which contain the particle in question, will be denoted $V_1, V_2, \dots, V_n$.

The change in the position vectors of the particle in two consecutive states is

$$l_i = r_{i+1} - r_i, \tag{2}$$

an elementary displacement of the particle.

The time interval θ_i during which the elementary displacement takes place is thus

$$\theta_i = t_{i+1} - t_i. \tag{3}$$

As the particle undergoes diffusive motion, an intermediate locally equilibrium state of free energy $F_i^{'}$ is formed between the pair of states with free energies F_i and F_{i+1}. The volume where this locally equilibrium state is formed is denoted $V_i^{'}$.

The difference in energies

$$E_i = F_i^{'} - F_i, \tag{4}$$

is usually referred to as a free activation energy.

In the diffusion motion the following condition is met

$$F_i^{'} > F_i, F_{i+1}. \tag{5}$$

As seen from the inequality (5), for the particle to undergo an elementary displacement, the system must overcome the energy barrier E_i. This occurs due to thermal fluctuations, and thus the transition from state with free energy F_i into the state with free energy F_{i+1} is referred to as the thermal fluctuation event. The state with free energy $F_i^{'}$ is referred to as an activated state and the states with free energies F_i and F_{i+1} as non-activated. Finally, the diffusive motion itself is a thermally activated motion.

Let's denote the lifetimes of states with free energies F_i and $F_i^{'}$ as τ_i and $\tau_i^{'}$, respectively. The lifetime of the elementary thermal fluctuation act, and thus the duration of the elementary displacement of the particle is determined by the following sum:

$$\theta_i = \tau_i + \tau_i^{'}. \tag{6}$$

According to Boltzmann's principle (Bagchi 2023), the following equation stands

$$\frac{\tau_i^{'}}{\tau_i} = exp\left(-\frac{E_i}{k_B T}\right), \tag{7}$$

where k_B is the Boltzmann constant and T is the absolute temperature.

The following inequality must also stand:

$$\frac{E_i}{k_B T} \gg 1. \tag{8}$$

With this in mind, equation (6) becomes

$$\theta_i \approx \tau_i. \tag{9}$$

In other words, the duration of the elementary displacement is the lifetime of the state with free energy F_i, or the lifetime of the equilibrium state between the displacements.

1.2. Diffusion of particles in hydrogel: a physical model

The general features of the diffusion mechanism in condensed matter, as mentioned above, should be inherent in the diffusion of foreign particles in a hydrogel. The free activation energy plays the main role in this mechanism (Wolde-Kidan et al., 2021). Within this mechanism, the fluctuation associated with the formation of the activated state, occurring in the region with the initial volume $V^{'}$, tends to increase with increasing volume. This tendency meets resistance from the environment. The amount of the resistance experienced must then determine the numerical value of the free activation energy. The polymer network of the hydrogel must significantly increase this resistance (compared to water) and thus must substantially increase the free activation energy.

For each position of the particle, the value of E_i is determined by many factors: the configuration of the polymer network in the vicinity of the particle, the network's rigidity, the particle's location relative to the network, etc. In other words, the value of E_i is determined by the local supramolecular structure of the hydrogel. The strict calculation of the free activation energy could be performed using methods of statistical physics. Instead, in the present work, we introduce a simplified thermodynamic model that accounts for the presence of the polymer network when describing the diffusion of foreign particles in a hydrogel. This model is based on approximations used in the classical diffusion theory (Frenkel, 1955).

The first approximation we use in the model is the following: we assume that the elementary displacements are equal in magnitude, and so are the durations of each elementary displacement. We denote the elementary displacements as l and the durations of these displacements as τ. Within such an approximation, the values of the diffusion coefficient must be a function of both l and τ:

$$D = D(l, \tau). \tag{10}$$

The unit of the diffusion coefficient, as indicated by (1), is $m^2 \cdot s^{-1}$. Based on this, the function in (10) is (up to a factor of order one) equal to:

$$D = {}^{l^2}/_{\tau}. \tag{11}$$

After substitution of (7) into (11) we get:

$$D = \frac{l^2}{\tau'} exp\left(-\frac{E}{k_B T}\right). \quad (12)$$

For the foreign particles in water (denoted by index "0") diffusion coefficient can be written as:

$$D_0 = \frac{l_0^2}{\tau_0'} exp\left(-\frac{E_0}{k_B T}\right). \quad (13)$$

The second assumption made in the model is that elementary displacements l and l_0 must be of the order of magnitude of the size of a particle, while τ' and τ_0' must be of the same order of magnitude (Frenkel, 1955). This implies that:

$$\frac{l^2}{\tau'} = \frac{l_0^2}{\tau_0'}. \quad (14)$$

Consequently, we can arrive at the following expression for the diffusion coefficient:

$$D = D_0 exp\left(-\frac{\Delta E}{k_B T}\right), \quad (15)$$

where

$$\Delta E = E - E_0. \quad (16)$$

According to (14), within the classical theory formalism, the presence of the polymer network changes the value of *D* as it changes the value of the free activation energy: ΔE.

Within the assumptions made, as indicated by expressions (10) and (14), ΔE must be the quantity averaged over the system. Therefore, it must be the function of macroscopic parameters, holistically characterizing the system. One of such parameters is the concentration q , a relative volume occupied by the polymer network.

Consequently, we assume the existence of a function of *q* which gives the values of ΔE:

$$\Delta E = f(q). \quad (17)$$

As the polymer network slows down the diffusion of the foreign particles, this function can be safely assumed to be monotonously increasing. In this case, we can expand this function into a power series and limit this expansion to the first term:

$$\Delta E = \left.\frac{df}{dq}\right|_0 q. \quad (18)$$

Then expression (15) becomes:

$$D = D_0 exp\left[-\frac{q}{Q(T)}\right], \quad (19)$$

where

$$Q(T) = \frac{k_B T}{\left|\frac{df}{dq}\right|_0}. \quad (20)$$

Expression (19) summarizes the essence of the model proposed. The presence of a polymer network changes the diffusion of the foreign particles via the change imparted on $Q(T)$. This quantity can be thought of as the value of concentration q that prevents the diffusion of foreign particles in the volume occupied by a hydrogel.

2. Materials and methods

In the present work, we used the following two gelling agents: agarose (purchased from Sigma-Aldrich) and gelatine (purchased from Bloom 200, France). Agarose is the main component (70–80%) of agar-agar natural extract obtained from *Florideophyceae* algae (Jiang et al., 2023). Gelatine is an animal-sourced protein, predominantly consisting of collagen. It can be found in animal skin, bones, and ligaments and is 90% protein (with such amino acids as glycine, proline, and hydroxyproline) (Milano et al., 2023). Both agarose- and gelatine- based hydrogels are bio-compatible. They have a porous structure (Lazarenko et al., 2025), that resembles a honeycomb structure, as revealed by cryo-scanning electron microscopy (Rahbani et al., 2013). Agarose pores are spherical in shape, with radii between 370 and 700 nm. Gelatine pores are smaller, more uniform, with radii between 320 and 650 nm. The foreign particles introduced into the hydrogel were rhodamine 6G (R6G) molecules. The hydrodynamic radius of the R6G molecule is only 0.65 nm (Majer, & Melchior, 2014), several orders of magnitude smaller than the size of the pores.

Unstained hydrogels were prepared by mixing gelling agents with distilled water and keeping them for 10 minutes at 90 °C. Hydrogels stained with a dye were prepared by mixing gelling agents with 0.1 % aqueous solution of R6G. The following samples were prepared: 2, 4, 6, 8 % agarose gels; 16, 20, 25 % gelatine gels; 10 % (2 % agarose + 8 % gelatine) and 14 % (4 % agarose + 10 % gelatine) mixtures.

The systems in which diffusion was observed were prepared as follows: first, 1 mL of pure hydrogel at 90 °C was placed in a 2 mL syringe. The hydrogel was allowed to cool to room temperature. Then 1 more milliliter of stained hydrogel at 60 °C was added to the syringe. The resulting sample with a boundary between the stained and unstained gel is shown in Fig. 1. Subsequent diffusion was observed in the syringe at 24 °C.

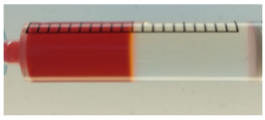

Fig. 1. Syringe with hydrogel at the beginning of the experiment: the left side contains rhodamine dye

To observe the diffusion process, the image processing analysis was utilized (Davydiuk et al., 2024). The syringe was uniformly illuminated with white, diffused light from two 40 cm – long rectangular white LED lamps, which were placed horizontally on a stand in front of a digital camera. The images were taken at equal time intervals, starting from the moment the stained and unstained hydrogels were brought into contact. The time intervals for hydrogels with higher concentrations were longer than for those with lower concentrations. The RGB images obtained were processed in ImageJ software. As R6G

absorbs blue light well, only the blue channel in the RGB image was used for processing and analysis. The changes in the blue channel intensity were normalized for each sample.

3. Results and their discussion

Figure 2 shows the snapshots of the syringes with hydrogels taken at 0, 2, 4, 6, and 14 hours after the start of the experiment. The rows of the figure represent the hydrogels with, respectively, 4 % (agarose), 8 % (agarose), and 16 % (gelatine) concentrations.

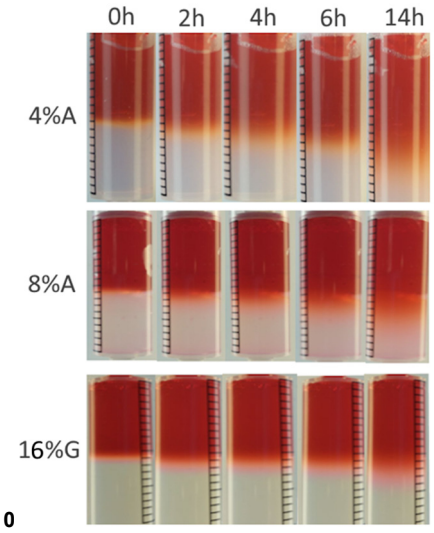

Fig. 2. Syringes with gels of different concentrations: 4 % (agarose), 8 % (agarose), and 16 % (gelatine). Images of the syringes were taken at the start of the experiment and after 2, 4, 6, and 14 hours, respectively

The initial analysis of Fig. 2 shows that the stained/unstained boundary moves more slowly for gels with higher R6G concentration. To quantify the diffusion rate, ImageJ was used. Firstly, the Image\Color\Split Channels function was used to split the RGB image into separate channels. Then, the blue channel image was converted to greyscale (Fig. 3 b).

The central section of the image was then selected for analysis using the Analyze\Plot Profile function (Fig. 3 c). This function was used to plot the intensity vs. coordinate function (Figure 3d), which correlates with the spatial distribution of the R6G relative concentration in the gel.

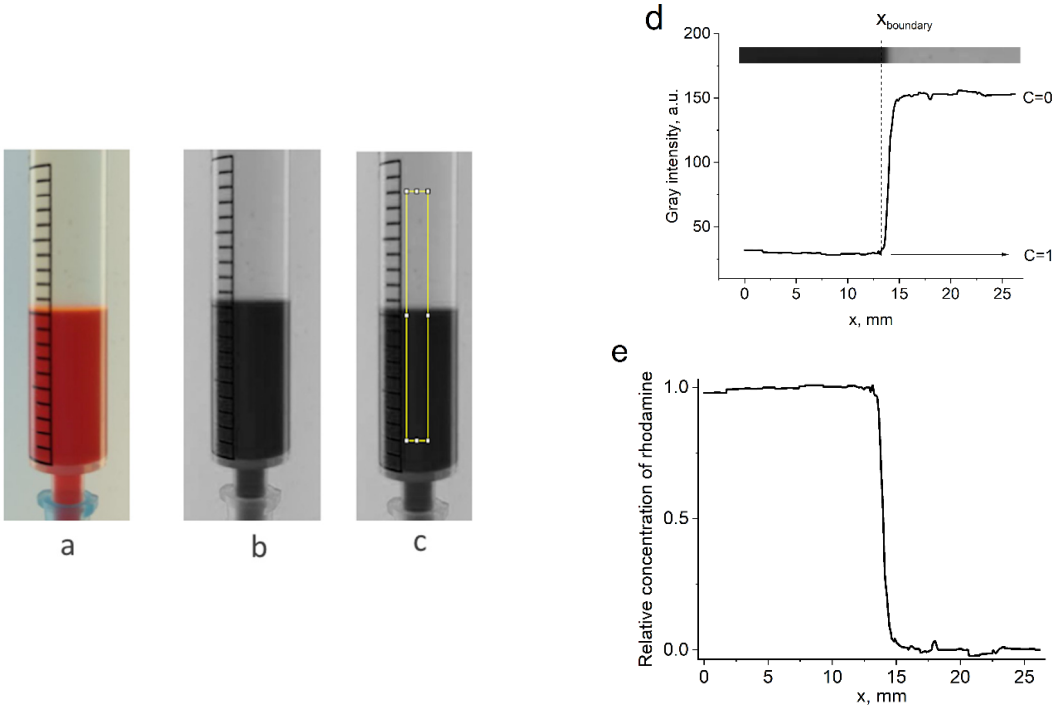

Fig. 3. Digitization of the images representing the dye concentration boundary (front) position in space. a – original image, b – the same image after converting into greyscale by blue color intensity, c – the area of the image used for the intensity distribution analysis, d – intensity of the greyscale image vs. coordinate, e – relative concentration of R6G vs. coordinate

In Fig. 3 e, the highest relative concentration (C) of R6G corresponds to $C = 1$, and the absence of R6G corresponds to $C = 0$. To determine the numerical value of the diffusion coefficient of the R6G in the hydrogel, a multistep algorithm was utilized. We use the data from Fig. 4, representing relative concentration vs. coordinate for the 25 % gelatine hydrogel, to illustrate this algorithm. The data in the graph shows the concentration of the dye at different points in the sample at different times.

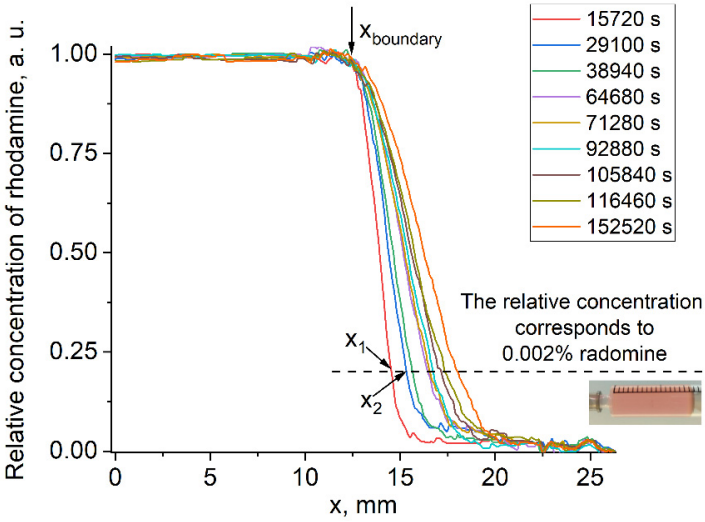

Fig. 4. Relative concentration of R6G vs. coordinate recorded at different times for the 25 % gelatine gel

The change in the concentration of R6G must obey Fick's second law (Crank, 1979):

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}, \tag{21}$$

where $C(x,t)$is the concentration of the substance that undergoes diffusion, D is a diffusion coefficient, $\frac{\partial C}{\partial t}$ is the partial first derivative of the concentration function with respect to time, whereas $\frac{\partial^2 C}{\partial x^2}$ is the second partial derivative of the concentration with respect to coordinate x.

The solution of (21) for a half-space with a constant concentration C_0 of the diffusant at the boundary is a Gauss error function (Crank, 1979):

$$C(x,t) = C_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right), \tag{22}$$

where x is the position of the boundary, and t is time.

Which gives the following expression:

$$D = \frac{{}^{x^2}/_{t}}{4\left(\mathrm{erfc}^{-1}\left(C(x,t)/C_0\right)\right)^2}. \tag{23}$$

To calculate the value of $\mathrm{erfc}^{-1}\left(C(x,t)/C_0\right)$ let's examine a gel with R6G concentration of 0.002 % (Fig. 4). The initial concentration of the rhodamine in the stained gel was $C_s = 0.1$ %. The boundary corresponds to the half of this value: $C_0 = C_s/2 = 0.05$ %. The 0.002 % concentration is thus 25 times smaller than that at the boundary. Such a value allows us to neglect the non-linear effects of a camera at high concentrations of the dye. The numerical value of the ratio $C(x,t)/C_0 = = 0.02$. The value of $\mathrm{erfc}^{-1}\left(0.02\right) \approx 1.453$.

Then the coefficient of diffusion is given by

$$D = 0.118\,{}^{x^2}/_{t}. \tag{24}$$

Expression (24) gives the value of the diffusion coefficient, given the position of the boundary at a given time instant.

In Fig. 4, a horizontal line corresponding to the given $(0.002\ \%)$ concentration of R6G intersects the graphs plotted for different time intervals at different values of coordinate x. The intersections provide the data point pairs x_1 and t_1, x_2 and t_2, and so on, corresponding to the same dye concentration. This data, x^2 vs. t is plotted in Fig. 5. As shown in this figure, the squared position of the given R6G concentration in a hydrogel appears to vary linearly with time, with a slope of $1.627 \cdot\cdot 10^{-4}\ mm^2 \cdot s^{-1}$.

Substituting this numerical value into the equation (24) we get the following for the diffusion coefficient: $D = 0.118 \cdot \cdot 1.627 \cdot 10^{-4} = 19.2 \cdot 10^{-6}\ \mathrm{mm^2 s^{-1}}$. The same algorithm is applied to determine the diffusion coefficient for gels with different gelling agent concentrations. This plot of diffusion coefficient vs. the concentration of a gelling agent in a hydrogel is shown in Fig. 6.

The variation of the diffusion coefficient with the concentration of the gelling agent appears to be exponentially decaying in agreement with (19) This behavior persists despite the different nature of the gelling agents – all points seem to fit the same curve, even though some of them correspond to agarose hydrogels, other to gelatine hydrogel, and the rest to hydrogels formed by the mixture of agarose and gelatine. The latter fact can be interpreted as follows: when the size of the diffusant molecule (R6G in this case) is much smaller than the pore size in the gel, the nature of the gel does not affect the diffusion coefficient.

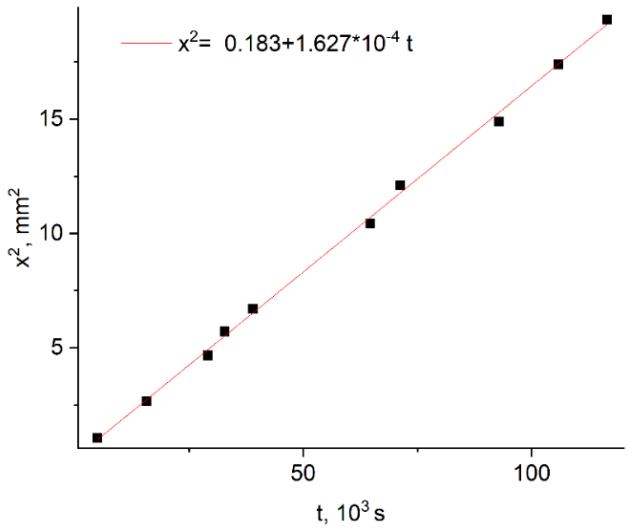

Fig. 5. Squared position of the given (0.002 %) concentration of R6G in a sample of 25 % gelatine hydrogel vs. time

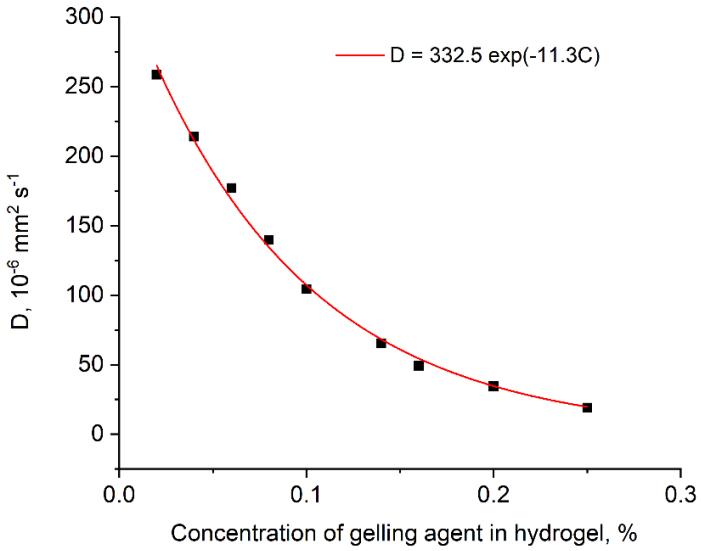

Fig. 6. Diffusion coefficient of R6G vs. gelling agent concentration in the hydrogel

Discussion and conclusions

The diffusive motion of foreign particles in hydrogels has features inherent to the diffusion of particles in any condensed matter. It can be thought of as a sequence of elementary displacements, in each of which the system, due to thermal fluctuations, overcomes an energy barrier called free activation energy.

Diffusion of foreign particles in the hydrogel is altered by the presence of a polymer network, which creates obstacles to the diffusion. Such interference forces the diffusion coefficient of the foreign particles to become a function of the relative volume occupied by the polymer network. This function has the form of an exponential decay. The constant that determines the rate of decay serves as a parameter characterizing the effect of the polymer network on the diffusion of foreign particles in the hydrogel.

The experiment shows that (within experimental uncertainty) this constant is identical for hydrogels of various natures. Thus, the exponential decay observed can be considered a universal process in polymer hydrogels. And latter fact may be of interest when engineering hydrogels intended for controlled drug delivery.

Authors' contribution: Yuri Zabashta – conceptualization; methodology; Yaroslav Lazarenko – investigation, formal analysis; Oleksandr Alekseev – investigation, conceptualization; Lena Vergun – investigation, writing – original draft; Kateryna Hnatuk – investigation; Dmytro Andrusenko – investigation, validation, formal analysis; Kateryna Yablochkova – Writing – review & editing; Roman Dinzhos – data curation, formal analysis; Neli Koseva – methodology, investigation; Maksym Lazarenko – investigation, validation, visualization, writing – review & editing, supervision.

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ВПЛИВ КАРКАСА НА ДИФУЗІЮ СТОРОННІХ ЧАСТИНОК У ПОЛІМЕРНИХ ГІДРОГЕЛЯХ

Запропоновано фізичну модель, що описує вплив каркаса на дифузію сторонніх частинок у полімерних гідрогелях. Під час побудови цієї моделі використано традиційний підхід, властивий класичній теорії дифузії в конденсованих середовищах. Отримано теоретичну залежність коефіцієнта дифузії від об'єму, зайнятого каркасом. Показано, що вплив каркаса на дифузію сторонніх частинок у гідрогелі визначається переважно змінами вільної енергії активації, викликаними наявністю каркаса.

За допомогою методу аналізу оптичних зображень отримано залежності коефіцієнта дифузії в гідрогелях агарози та желатини з різною концентрацією гелеутворювача. Встановлено, що отримані експериментальні залежності узгоджуються з теоретичною залежністю, передбаченою запропонованою фізичною моделлю. Показано, що коли розмір часток дифузанту набагато менший від розміру пори гідрогелю, то коефіцієнт дифузії зележить не від природи гідрогелю, а від концентрації гелеутворювача.

К л ю ч о в і с л о в а : ***дифузія, гідрогелі, агароза, желатин, родамін, полімерна сітка.***

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