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COMPUTER MODELING OF BIOLOGICAL CONTAMINANTS IN A TRACK BIOSENSOR

Abstract. Many solids in biology, medicine and technology are porous materials into which impurity solutions are capable of penetrating. Concerning the pore population, one has to distinguish on the one hand, between open and closed pores, and on the other hand, between macroscopic and nanoscopic pores. Open pores are accessible from the surface by non-diffusive capillarity percolation processes or micro-capillary diffusion; closed pores that do not have any direct connection to the outside world are accessible from the outside only by diffusion. The transition from macroscopic (where fluid dynamics and capillarity hold) to nanoscopic (where nanofluidics holds) pores takes place when the pore radius is of a similar magnitude to the Debye length.

Creation of sensor systems for detecting extremely low concentrations of biological contaminants in liquid media is the most important task of bio-nanotechnologies. Since such systems are in great demand, it is necessary to find ways to make such devices as cheap and simple as possible while ensuring their high sensitivity. In this work, using computer simulation, we demonstrate the possibility of creating biosensors based on the use of measurements of the simplest physical characteristics. It is shown that the sizes of particles that pollute the environment and their charge can serve as discriminating parameters that allow one to detect the presence of such particles. To conduct a computer experiment, a model of a track biosensor was developed.

Key words: biological contaminants, nanopores, ion flows, biosensors

INTRODUCTION

There are quite a number of strategies to use swift heavy ion tracks for producing biosensors [1, 2]. The pore blocking concept is introduced by Siwy et al. [3]. In order to maximize the sensing effect a reaction for detection biological contaminants should preferentially take place in confinement, such as given within very long and very narrow etched track [4]. The simulation of diffusion processes in nanotrack was performed [5]. This simulation was based on the simplifying assumption that, in spite of the nanometer-sized etched tracks, nanofluidic effects do not play any role in this case (the validity of this assumption is examined in greater detail in the work [6]).

In this work, we used the nanotrack model described in [1]. However, additional improvements to the model made it possible to identify ways to improve the service parameters of track biosensors. The computer program algorithm takes into account the possibility of changing the size of model particles, provided that their density is maintained. Another feature of the modified algorithm is the ability to take into account the Coulomb interaction not only between model particles, but also between particles and adsorption centers. Implementation of such an algorithm in a computer experiment required improvement of the adsorption center model.

An improved computer model of the nanotrack made it possible to take into account the simultaneous difference in the size and charge of particles simulating pollution from the corresponding characteristics of the main substance. It was important to take into account the ratio of these parameters in the interaction of model particles with adsorption centers and scattering centers on the inner surface of the track. The mechanism of detecting bio-contaminants in the track biosensor is associated with the complex interaction of the impurity (contaminant) component of the flow with defects in the inner surface of the track [1]. Therefore, it was important to elucidate the effect of different combinations of these parameters on changes in the current density in the nano-channel.

DESCRIPTION OF AN ADSORPTION CENTER

To optimize the parameters of the track biosensor, it is necessary to achieve certain characteristics of adsorption centers on the inner surfaces of the track. The flow of a substance passing through a track is retarded due to the fact that individual particles are "retained" in potential wells of adsorption centers. The time spent by the particle in the potential well of the adsorption center (and hence the time of "delay" of the particle when moving in the track) depends on the depth of the potential well. According to the adsorption center model described in [7, 8], the depth of the potential well is proportional to the Hooke coefficient. The center is a hole in the track surface, formed by the absence of two, three or four ions in the "wall" of the track. The ions moving inside the track under the action of an external force are attracted by the Coulomb field of the center and penetrate into the hole of the center due to the acquired velocity.

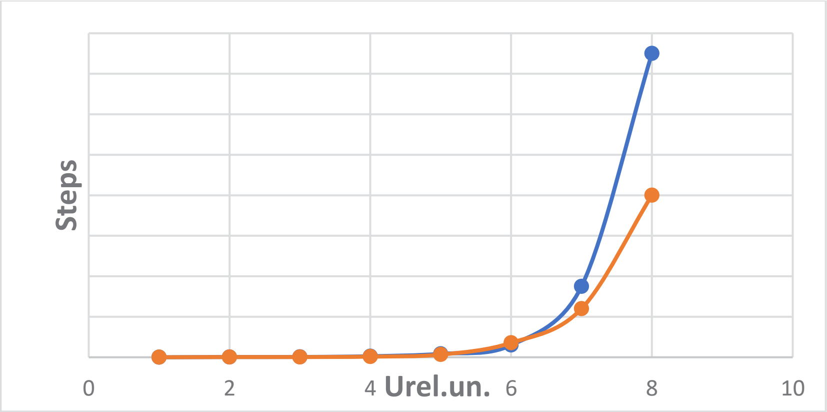

Fig. 1. Dependence of the lifetime of a model particle in a potential well on the depth of the well, the red curve corresponds to a larger value of the applied voltage

The result, shown in Fig. 1 gives the average value of the lifetime of a model particle in the potential well, obtained for the three studied shapes of holes that form the potential well of the center. A characteristic feature of the result in Fig. 1 is that, in contrast to the usual exponential dependence, a curve with a sharp rise is obtained. This means that adsorption centers begin to affect significantly the flux density of the carrier substance at a sufficiently deep potential well.

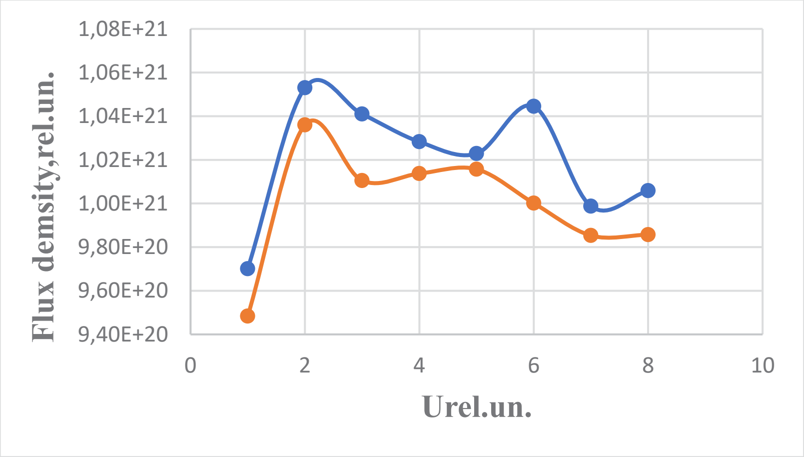

Fig. 2. Dependence of the flux density of the carrier substance on the depth of the potential well of the adsorption center; curves of different colors correspond to two randomly selected adsorption centers

Fig. 2 shows that the current density of the carrier substance is not determined unambiguously by the value of the binding energy of adsorption centers, which could be concluded based on Fig. 1. A computer experiment confirms that the charge of adsorption centers significantly affects the current density across the track, but a detailed study of other factors is required in order to unambiguously establish a correlation between the presence of a certain amount of bio-contaminants and the current density.

DETECTION OF INDIVIDUAL "BACTERIA"

In [7] it was found that in the case of inclusion in the flow of model particles of one particle, which differs from the main flow in large dimensions (let us conventionally call it a "bacterium", Fig. 3), the current density experiences a sharp negative peak. The time dependence of the ion current density in the nanotrack is a pulsating line [8].

Next, a computer experiment was carried out with the introduction of "bacteria" into the ion flow at certain time intervals (the number of integration steps). The time between the moments of introducing the next "bacterium" into the ion flow was changed. It turned out that there is a critical time interval (the number of integration steps) less than which not all "bacteria" that have already appeared in the flow are fixed. Thus, it becomes possible to introduce the concept of sensor resolution. It is important in the process of creating a sensor to work out the detection of "bacteria" at the initial stage of their appearance. It is also important to take the necessary action before accumulating the amount of bacteria corresponding to the "sensing quorum" [9].

In the case of a time interval of less than 1000 steps, the second "bacteria" was not always fixed. As the interval decreased, the probability of fixation of both bacteria simultaneously decreased.

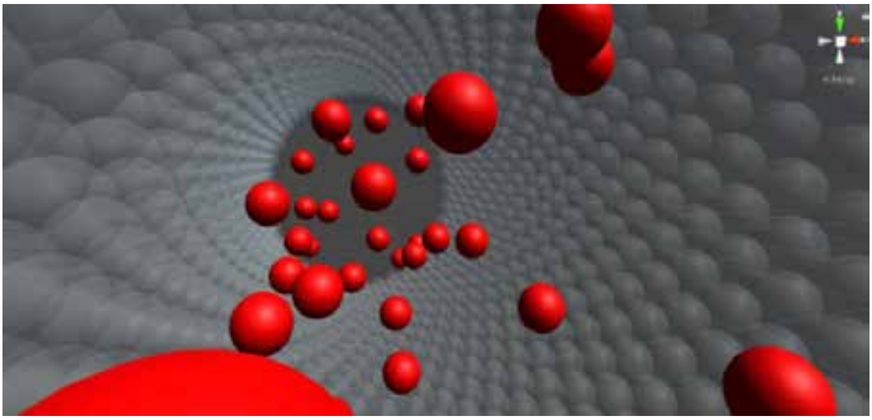

Fig. 3. The model particles of larger sizes as bio-contaminants into the ion flow. In the Figure one sees the particles from the top section of track along its axis

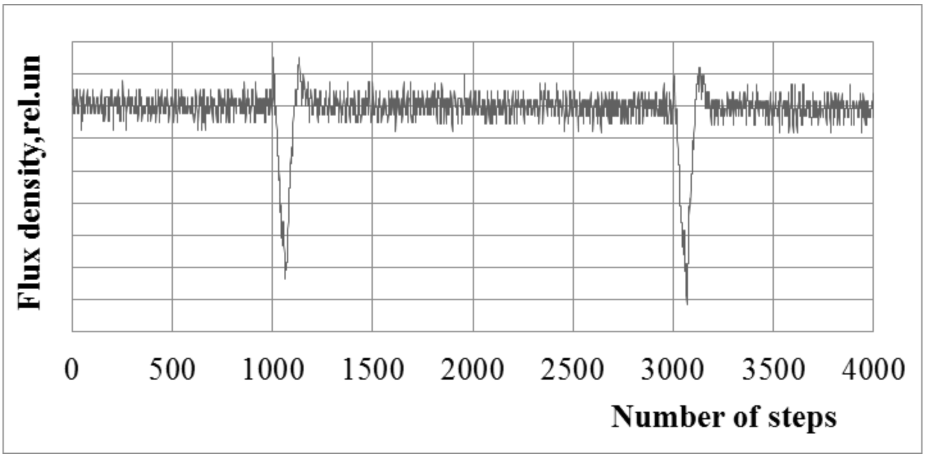

Fig. 4. Fixation of two "bacteria" that entered the ion flow with an interval of more than 1000 steps

Next, a computer experiment was carried out with the introduction of different amounts of "bacteria" into the ion stream with different intervals between the introductions of subsequent "bacteria" (see, for example, Fig. 5 and Fig. 6).

On Fig. 5 it is shown that all 4 "bacteria" appeared when the interval between their introductions was more than 500 steps, and on Fig. 6 all 17 "bacteria" appeared at an interval of more than 150 steps.

In this study, we considered bio-contaminants in the form of model particles, the size of which exceeds the size of the carrier flow ions. Therefore, the results obtained are valid when size is the discriminating factor for specific bio-contaminants. If these sizes turn out to be smaller than the particle size of the carrier flow, then the results can be significantly different.

Note that in our case (for the indicated sizes of pollutant particles), the density of the total flow of the carrier substance with pollution decreases with an increase in the content of pollutant particles. This is illustrated in Fig. 7.

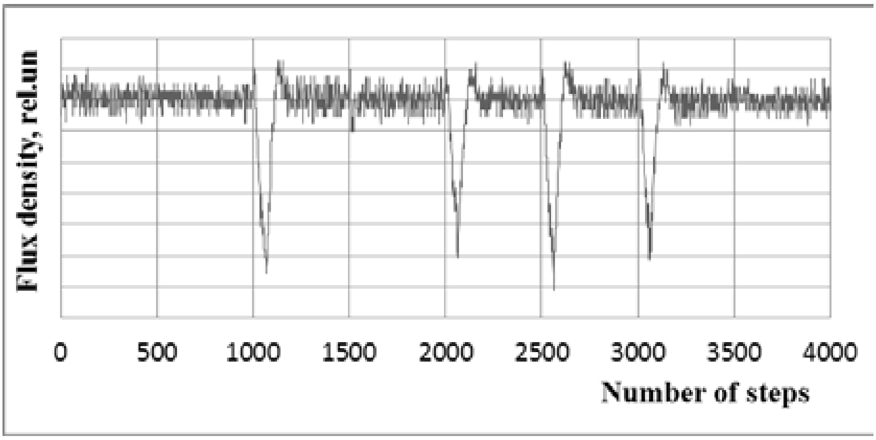

Fig. 5. Fixation of four “bacteria” that entered the ion flow with an interval of more than 500 steps

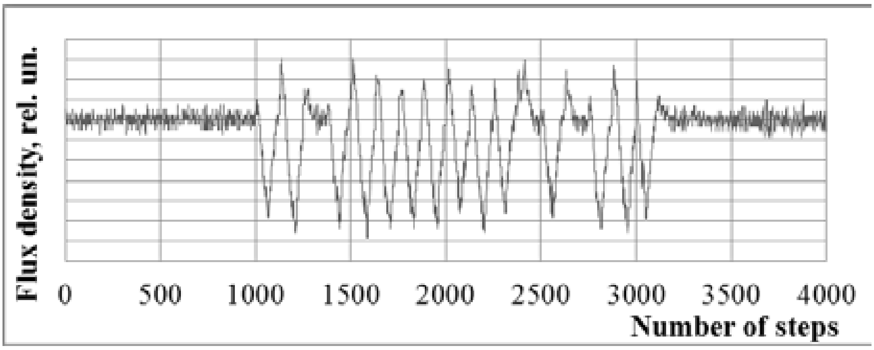

Fig. 6. Fixation of seventeen “bacteria” that entered the ion flow with an interval of more than 150 steps

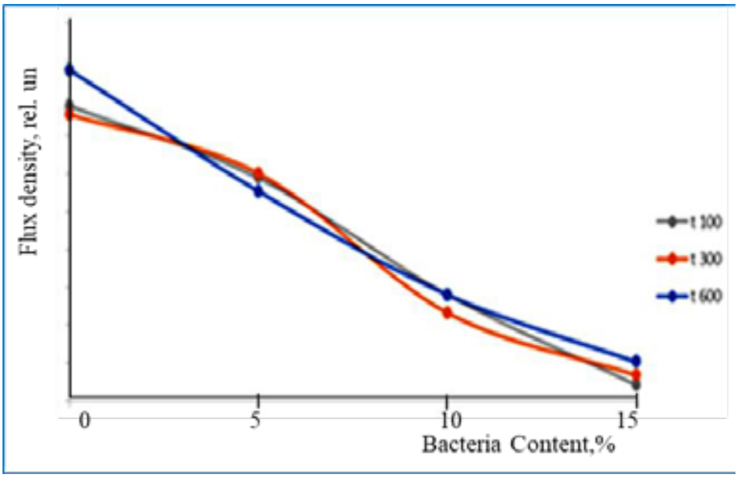

Fig. 7. Dependence of the total flow through the nanotrack (including contaminants) on the concentration of contaminants

DISCUSSION

The functioning mechanisms of various types of biosensors are mainly based on the use of complex chemical reactions and electron-lattice interactions [10, 11]. Therefore, an urgent task is to create sensor systems capable of detecting pollution based on measurements of simple characteristics of pollution, including biological ones. These can also be living organisms (bacteria), which differ, for example, from the particles of the studied medium in size. Track structures can be used to create such sensors. With this approach, instead of one complex and long instrument, a series of simple and relatively cheap instruments can be created.

With this approach, it will be possible, by solving certain design problems, to create a device that combines simpler devices, which will be more economical and which will be easier to operate.

The magnitude of the negative peaks in Fig. 4 depends on the particle size ratio of the main substance and the polluting particles. The peaks arise as a result of the elastic interaction of spherical model particles. The appearance of particles of a different size in the system changes the particle velocity distribution. These effects depend on the temperature of the particles as well as on the external applied force (applied voltage).

CONCLUSIONS

The passage of a current of an inhomogeneous ionic liquid through a nanotrack was studied by computer simulation. The possibility of using such a system as the basis of a track biosensor has been established. Thus, a simplification of the biosensor design is achieved, and a new approach to the creation of simpler and cheaper sensor systems can be implemented.

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АНОТАЦІЯ

КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ БІОЛОГІЧНИХ ЗАБРУДНЕНЬ У ТРЕКОВОМУ БІОСЕНСОРІ

Багато твердих речовин у біології, медицині та техніці є пористими, через пори різного діаметру можуть проникати розчини домішок. Стосовно класифікації пор, слід розрізняти, з одного боку, відкриті та закриті пори, а з іншого боку – макроскопічні та наноскопічні пори. Відкриті пори доступні з поверхні за допомогою недифузійних процесів капілярної перколяції або мікрокапілярної дифузії; закриті пори, які не мають прямого зв'язку із зовнішнім світом, доступні ззовні лише шляхом дифузії. Перехід від макроскопічних (де зберігається динаміка рідини та капілярність) до наноскопічних (де зберігається нанофлюїдика) пор відбувається, коли радіус пори має подібну величину до довжини Дебая. Створення сенсорних систем для виявлення надзвичайно низьких концентрацій біологічних забруднень у рідких середовищах є найважливішим завданням біонанотехнологій. Оскільки такі системи користуються великим попитом, необхідно знайти способи зробити такі пристрої максимально дешевими і простими, забезпечуючи при цьому їх високу чутливість. У даній роботі за допомогою комп'ютерного моделювання продемонстровано можливість створення біосенсорів на основі використання вимірювань найпростіших фізичних характеристик. Показано, що розміри частинок, які забруднюють навколишнє середовище, та їх заряд можуть бути дискримінаційними параметрами, які дозволяють виявити наявність таких частинок. Для проведення комп'ютерного експерименту була розроблена модель трекового біосенсора.

Ключові слова: біологічні забруднення, нанопори, іонні потоки, біосенсори.