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ABSTRACT

The study concerning nano-scale systems is considered to highly contribute to the developments in the field of nano-technology where many models have been proposed in the literature. The information is carried by molecules in the diffusion medium of the models. Channel parameters such as the diffusion constant are very important for communication of the molecules between the transmitter and the receiver. The physical properties of the carriers and the density of the medium are also very important for the transfer of information. In this study, the number of received molecules is analyzed with respect to the environmental parameters of the channel such as viscosity and the diffusion constant. First, the diffusion constant is obtained analytically by using the Stokes–Einstein equation, and then a new model was developed in Matlab and analyzed in terms of performance of the system concerning channel parameters such as the diffusion constant. Second, the diffusion constant of the medium was predicted by using an artificial neural network and compared with the simulation results. The different diffusion constant values have been used in the environment contrary to the literature to obtain the number of received molecules. The predicted values of the number of received molecules for D = 75 $\mu m^2/s$ and D = 150 $\mu m^2/s$ were also obtained for mobile and fixed system models. The difference between predicted and simulation values is obtained as ±0.5 by using residual analysis.

I. INTRODUCTION

The number of current densities that can be an atom, hole, electron, and molecule determines the current, that is, the rate of charge flow in the medium. The current flow can also be calculated since it is known as the number of charge carriers. There are two current mechanisms—drift and diffusion—that make the charges to move. A charge moves under the influence of an electric field since the applied field exerts a force[1]

$$F = qE, \tag{1}$$

on the charge carriers, where E and F represent the applied field and force, respectively. This movement results in a current, which is known as the drift current,

$$I_d = nqV_dA, \tag{2}$$

where I_d, V_d, A, n, and q are the drift current, drift velocity of the charge carrier, area of the medium, number of charge carriers per unit volume, and charge of the electron, respectively. The mobility carrier, μ, can be measured based on how easily charge carriers move under the influence of an applied field or can be determined based on how mobile the charge carriers are,[1]

$$\mu = \frac{V_d}{E}. \tag{3}$$

If the medium is at thermodynamic equilibrium (there is no applied field), the carrier has a thermal energy of $\frac{k_BT}{2}$ for 1D (one dimensional), and the thermal energy and velocity of the electron for 3D (three-dimensional) environments are given below:

$$E = \frac{3k_BT}{2} \text{ and } V_{th} = \sqrt{\frac{3k_BT}{m^*}}, \tag{4}$$

where V_{th}, k_B, m^*, and T refer to the thermal velocity of the electron, Boltzmann constant (1.38×10^{-23} J/K), and effective mass and temperature of the medium (Kelvin), respectively. If there is no applied field, the movement of the molecules will be completely random, and this randomness causes no net current flow. Molecules move in the system due to their thermal energy or applied field, but they collide with each other. The average time taken between collisions is called relaxation time or mean free time τ. Hence, we can define mobility as

$$\mu = \frac{q\tau}{m^*}. \tag{5}$$

Diffusion current is defined as the movement of the carriers from the high concentration region toward the low concentration region.[2] As the carriers diffuse in the fluid environment, a diffusion current flows. The force behind the diffusion current is the random thermal motion of carriers. A concentration gradient produces a pressure gradient that also generates the force on the molecules, making them to move.[1] According to the electrical mobility equation, the diffusion constant (D) for charged particles is defined as follows:

$$D = \frac{\mu k_B T}{q}. \tag{6}$$

The diffusion process causes the substance concentrations in a system to equalize or occurs by the distribution of an equilibrium concentration resulting from the random movement of the system elements.[2,3] If nano-/micro-scale particles have stayed in a liquid at rest, they unsystematically move from one part of the bulk to another; the motion of the particle does not decrease, and it is independent of the chemical properties of the medium. This event is known as Brownian motion.[4]

In Fick's first law, the diffusion flux is related to the gradient of concentration, so the gradient goes from high to low concentration regions. The most common assumption is Fick's law,

$$J = -D\frac{d\varphi}{dx}, \tag{7}$$

where J, D, φ, and x are the diffusion flux, diffusion coefficient, and concentration and position of the molecules, respectively.[5]

Einstein showed that the diffusion coefficient D in an infinitely dilute solution is given by the equation

$$D = \frac{k_B T}{f}, \tag{8}$$

where f is the frictional coefficients of the particle. While the value of f, in general, is unknown, Charbonneau[6] showed that for the special case of a spherical particle of radius R_B, which is moving with a uniform velocity in a continuous fluid of viscosity η, the frictional coefficient f is given by

$$f = 6\pi\eta R_B. \tag{9}$$

It is known that the transfer of information generally takes place in the form of free diffusion movement of molecules in the environment. The feature of the transmission medium is determined with the diffusion coefficient; D for the diffusion of spherical uncharged particles through a liquid is given below.[1] Breki and Nosonovsky[7] pointed out that if one can assume that this equation also applies to spherical molecules, then their diffusion coefficients should be given by the equation

$$D = \frac{k_B T}{6\pi\eta r}. \tag{10}$$

As given in the formulas mentioned above, the definition of the viscosity and diffusion constant is briefly explained, and the diffusion constant and viscosity are observed to be inversely proportional.

First, the effect of diffusion constant, which is an important part of the environment of nano-scale systems (NSSs), is analyzed in detail in Matlab in the present study. In the literature, the general hitting probability of the transmitted molecules is analyzed at the receiver part using some system parameters such as the distance between the transmitter and the receiver, diffusion constant, and receptor deployment on the receiver.[8–12] Hitting probability of a transmitted molecule in 1D and 3D environments is as follows:

$$f_h^{1D}(d,t) = \frac{d}{\sqrt{4\pi D t^3}} e^{\frac{-d}{4Dt}} \tag{11}$$

and

$$f_h^{3D}(d,t) = \left(\frac{r_x}{r_x + d}\right) \frac{d}{\sqrt{4\pi D t^3}} e^{\frac{-d}{4Dt}}, \tag{12}$$

where D, r_x, and d show the diffusion constant, the radius of the receiver, and the distance from the transmitter to the receiver, respectively.

In nano-scale systems, to send information from the transmitter to the receiver or vice versa, chemical transceiver systems could be more favorable because of implementation issues. These models can be used in many areas such as for dentistry, bio-medical, environmental monitoring, industrial, and defense purposes. Receptors are almost used by all biological cells at their receiver surface to receive proteins, nutrients, or other substances.[10,13,14]

A lot of studies have been carried out on the analysis of nano-scale systems in recent years.[15–17] The transmitter (T_x) and receiver (R_x) parts are investigated to analyze transmitted and received molecules in fluid media. However, generally, the R_x entity and the received signal are considered to analyze NSSs. For example, the channel transfer function with a point transmitter and fully absorbing spherical receiver formulation for molecular communication via diffusion is introduced in Ref. 18.

Valincius *et al.* proposed a model with a point transmitter and a perfectly absorbing spherical receiver, which can move randomly in any of the three coordinates. The closed form expression is derived for the expected hitting rate by using three-dimensional unlimited communication channels for mobile nano-machines. The molecular communication channels mainly have two categories which are pure diffusive channels where the molecules move only due to the concentration gradient between the two regions. The flow of information molecules inside the pure diffusive medium uses the Brownian motion. The second channel model is the flow-based diffusive channels, where the displacement of molecules depends on the flow of the fluid with diffusion. The communication of nano-machines comes true via diffusion of the information molecules through the probability of information molecules at the receiver part. Hence, the mobility of nano-devices and its effect on the end-to-end performance of diffusive molecular communication are analyzed.[19]

In the second part of this study, one of the system parameters, the diffusion constant, is examined by using the Artificial Neural Network (ANN) algorithm in Matlab. The diffusion constant is simulated and predicted by using the ANN, and the results were also compared with the results of the proposed NSS model.

In recent years, researchers have tried to develop a model of the neuron that exists in the brain, and they call it an artificial neural network. Artificial neural networks are developed by using a nerve cell, which is known as the neuron of the living. An ANN consists of an input, hidden layer, and output. A fairly simple and small-sized ANN has some powerful features in information and information processing, even compared to its similarity to the human brain. The ANN is used by researchers for engineering applications increasingly because of the easy ability to learn directly from target outputs. Moreover, the ANN can adapt and solve the problem according to new data.[20] Therefore, for engineering applications, the ANN can be used as an effective tool[17,20–26] for NSS networks.

The rest of the paper is organized as follows: In Sec. II, the proposed system model is explained. In Sec. III, results of the proposed system model are given. Finally, Sec. IV concludes the paper.

II. SYSTEM MODEL

The number of hitting molecules until time t, for 1D and 3D environments, is given below:

$$N_{hit}^{1D}(t) = erfc\left(\frac{d}{\sqrt{4\pi Dt}}\right), \tag{13}$$

$$N_{hit}^{3D}(t) = \left(\frac{r_x}{r_x + d}\right) erfc\left(\frac{d}{\sqrt{4\pi Dt}}\right), \tag{14}$$

where $erfc$, d, and r_x refer to the error function, distance between the transmitter and the receiver, and radius of the receiver, respectively.

The NSS model shown in Fig. 1 consists of a point transmitter and mobile receiver and information molecules and receptors placed on the receiver. The shape of the receiver is chosen as a sphere in this study while the transmitter is assumed to be a single point in space. Messenger molecules are used as the information carriers between the transmitter and the receiver. First, the receiver is placed at the origin (0, 0, 0), and the transmitter is placed at a distance d from the receiver; then at every time step of the simulation, positions of the transmitter and the receiver are changed randomly for the mobile system model. The transmitter and the receiver both reside in a fluid propagation medium. It is assumed that the medium is unconfined, thus extending to infinity in all directions. After the molecules are released to the medium where they diffuse according to Brownian motion, they probabilistically arrive at the receiver. In this study, receptors which are placed randomly on the receiver are also considered to analyze the system model. The spherical receiver uses its receptors with a radius of r_s to absorb the information molecules. If a molecule collides with one of the receptors deployed on the surface of the receiver, it is absorbed by the receiver. If it collides with the surface of the receiver without touching a receptor, it bounces back.[10]

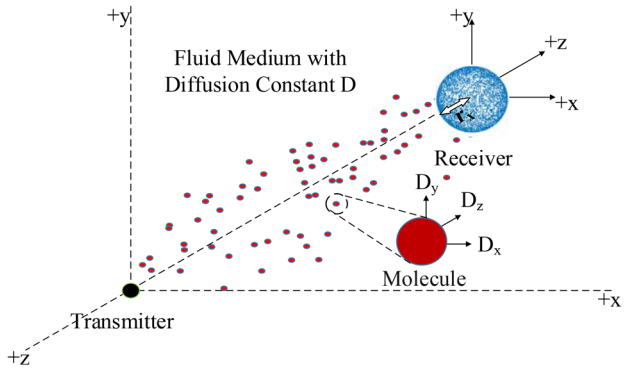

FIG. 1. Proposed model with a point transmitter and a spherical receiver where molecules and the receiver move randomly in the fluid environment with a different diffusion constant of D.

The diffusion process can be simulated via Monte Carlo simulations in the literature.[27] In a three-dimensional (3D) free diffusion molecular channel, the displacement at each dimension in Δt duration follows a Gaussian distribution, and the displacement vector is added to the location vector for evaluating the next position of a molecule.

After each propagation step, molecules are checked for reception considering the receptors on the receiver. For a spherical fully absorbing receiver, the cumulative number of received molecules is derived analytically. For a molecule in transition, the absorption probability by the fully absorbing receiver until time t is given in Eq. (14).

III. RESULTS AND DISCUSSION

A. System parameters

The number of received molecules based on simulation and analytical models was observed, and system parameters used in the proposed models are given in Table I.

These parameters are used for analytical and simulation results by using Eq. (14).

B. Fixed receiver model

In this model, first, the diffusion constant of the medium and the position of the receiver and the transmitter are kept constant. The probability of absorbing the mobile molecules from the receiver was obtained by simulation and analytically as illustrated in Fig. 2. Simulation and analytical results are almost similar concerning the number of received molecules.

TABLE I. System parameters.

Symbol	Quantity	Value
D	Diffusion constant	79.4 $\mu m^2/s$,
r_s	Radius of the receptor	0.01 μm
$N_{receptor}$	Number of receptors	7200
d	Distance between the receiver and the transmitter	5 μm
N_{Tx}	Number of molecules	20 000
	Number of simulations	100

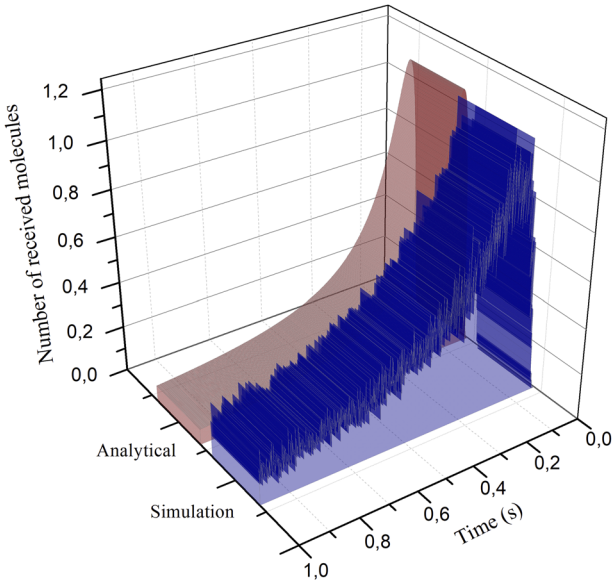

FIG. 2. Number of received molecules versus time for analytical and simulation results using a fixed receiver at D = 79.4 $\mu m^2/s$.

After that, the diffusion constant of the medium was changed between 50 and 200 $\mu m^2/s$ for a fixed receiver and transmitter model as shown in Fig. 3. As the diffusion constant increased, the number of the received molecules was also raised as expected. With an increasing diffusion constant, the viscosity of the medium was decreased because the mobility of molecules rose. Therefore, the number of received molecules is also increasing, and it is confirmed by Eqs. (6) and (10).

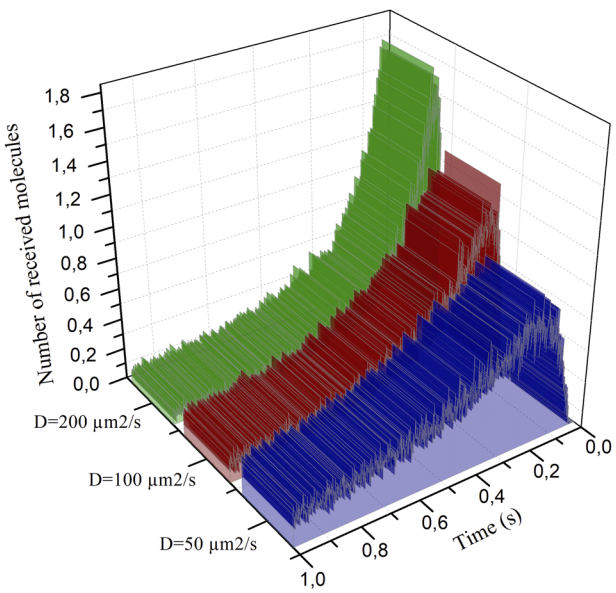

FIG. 3. Number of received molecules vs time using D values of 50, 100, and 200 $\mu m^2/s$ for the fixed receiver model.

C. Mobile receiver model

For the mobile receiver model, the probability of receiving molecules was analyzed by simulation and analytically. The diffusion constant was kept constant, and the transmitter and the receiver were mobile. As seen in Fig. 4, the simulation and analytical results are similar to each other, but it is observed that the number of received molecules in the analytical result is higher than that in the simulation result. Because analytic formulas for the mobile receiver system model are given without considering the receptors on the receiver,[28,29] in this model, the receptors are considered analyzing the model.

The number of received molecules by changing the diffusion constant of the medium was examined in the mobile receiver model as shown in Fig. 5. Similar to the fixed receiver model, it was observed that as the diffusion constant increases, the number of received molecules also increased as expected.

D. Comparing the fixed and mobile receiver model

The number of received molecules obtained using the same diffusion constant of the mobile and fixed receiver models is shown in Fig. 6. In the model where the receiver is mobile, it has been observed that the number of receiving molecules is higher. The probability of receiving molecules depending on the distance between the receiver and the transmitter is confirmed with Eq. (12). Therefore, the mean distance between the transmitter and the receiver in the mobile system is smaller than that in the fixed system; the number of the received molecules is also greater.

E. Artificial neural network

The machine learning techniques that simulate the learning system of biological organisms are commonly used and known as

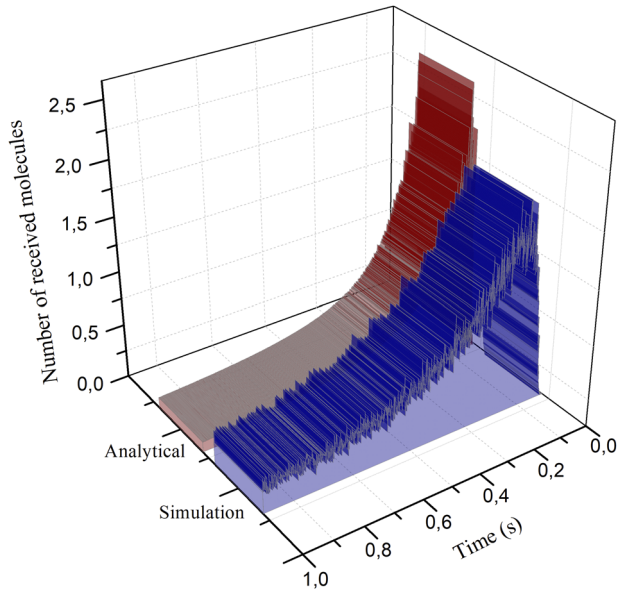

FIG. 4. Number of received molecules versus time for analytical and simulation results using a mobile receiver at D = 79.4 $\mu m^2/s$.

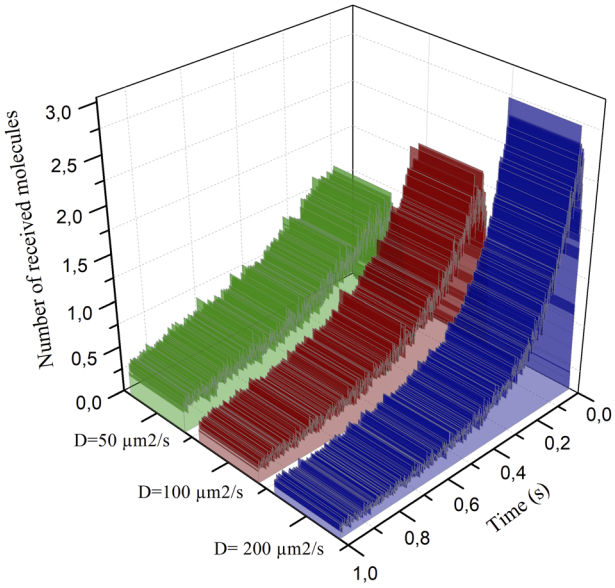

FIG. 5. Number of received molecules vs time using D values of 50, 100, 200 $\mu m^2/s$ for the mobile receiver model.

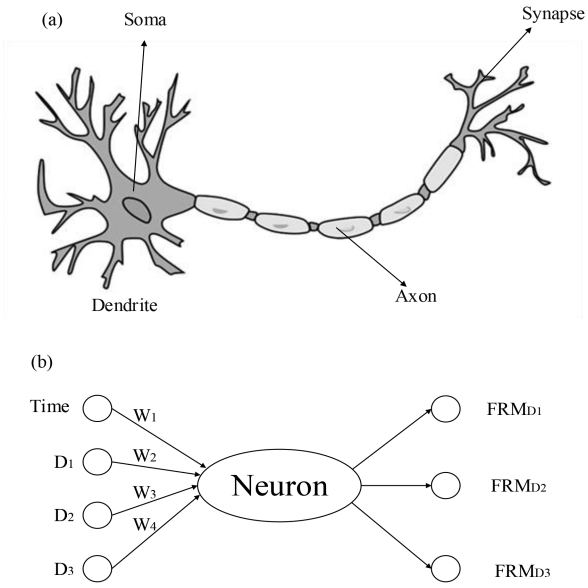

FIG. 7. (a) Biological neural network and its Matlab architecture: (b) the artificial neural network with 4 inputs, 3 outputs, and one hidden layer.

artificial neural networks.[30,31] The human being's nervous system implicates cells that are referred to as neurons. The system that allows neurons to connect is called axons, or dendrites, and the junction areas formed between dendrites and axons are known as synapses. These systems are illustrated in Fig. 7(a).

After obtaining the simulation result of the number of received molecules, the prediction was performed by using the ANN model that is developed in Matlab 2020b with an Intel(R) Core(TM) i7-1065G7 central processing unit (CPU) @ 1.30, 1.50 GHz, 16 GB Ram, 512 GB SDD, Windows 10 Home edition and ×64-based system. According to simulation data, 4 × 1000 inputs, one hidden layer with ten neurons, and 3 × 1000 outputs are used for the system model of the ANN. Matlab architecture of the proposed ANN model is also shown in Fig. 7(b). In this model, inputs are chosen as D_1 (D = 50 $\mu m^2/s$), D_2 (D = 100 $\mu m^2/s$), D_3 (D = 200 $\mu m^2/s$), and time. Outputs are also chosen as fraction of received molecules (FRM) (FRM_{D1}) (number of received molecules of D_1), FRM_{D2} (number of received molecules of D_2) and FRM_{D3} (number of received molecules of D_3). In this model, network type, transfer function, initialization of the weights, training function, adaption learning function, performance function, and the number of layers are chosen as the feed forward back propagation algorithm, Tansig, Sigmoid, Trainlm, Learngdm Mean Squared Error (MSE), and R^2 are used for training the proposed ANN model. The optimization process is also chosen as the Levenberg–Marquardt algorithm in this study.

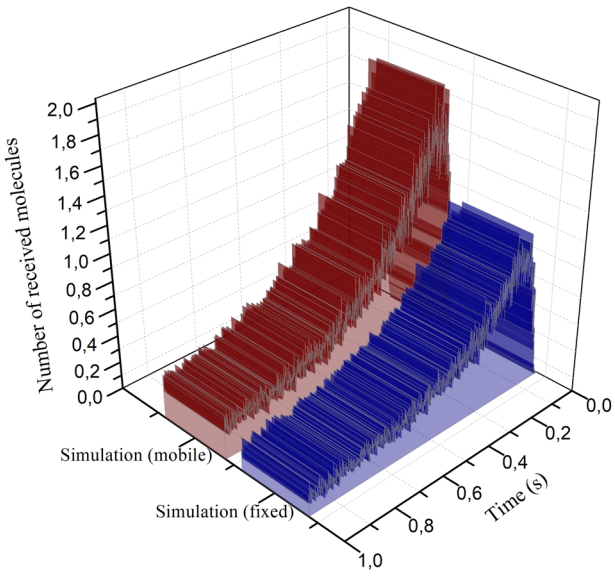

FIG. 6. Number of received molecules versus time for simulation results using the mobile and fixed receiver models at D = 79.4 $\mu m^2/s$.

In this part of the study, the number of received molecules is predicted using the ANN model for diffusion constants of 75 and 150 $\mu m^2/s$. For the proposed ANN model, 70% of the data were used for training, and 30% were used for testing. The performance criteria of the proposed method were evaluated according to the coefficient of determination (R^2) and Mean Squared Error (MSE) techniques. The coefficient of determination (R^2) and Mean Squared Error (MSE) techniques are used to compare obtained results. Formulation of MSE and R^2 is given in the following equations:

$$MSE = \frac{\sum_i (AnalyticalValue_i - Sim_i)^2}{N}, \tag{15}$$

$$R^2 = 1 - \frac{\sum_i (AnalyticalValue_i - Sim_i)^2}{\sum_i (Sim_i)^2}, \tag{16}$$

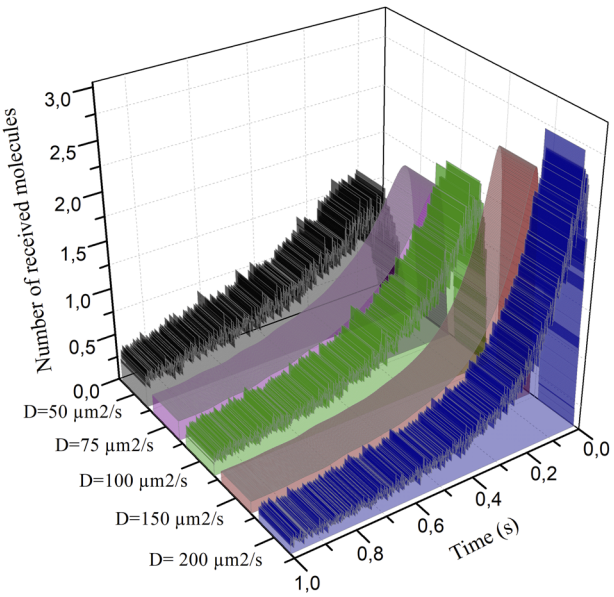

FIG. 8. Number of received molecules vs time using D values of 50, 100, and 200 $\mu m^2/s$ for simulation results and D values of 75 and 150 $\mu m^2/s$ for predicted results of the mobile system with the ANN.

where Analytical Value, Sim, and N refer to the value of analytical data, the value of simulated results, and the number of samples in the proposed model, respectively. The coefficient of determination and MSE are expected to become around 1 and 0 correspondingly. Although R^2 values are obtained around 1 for training and testing

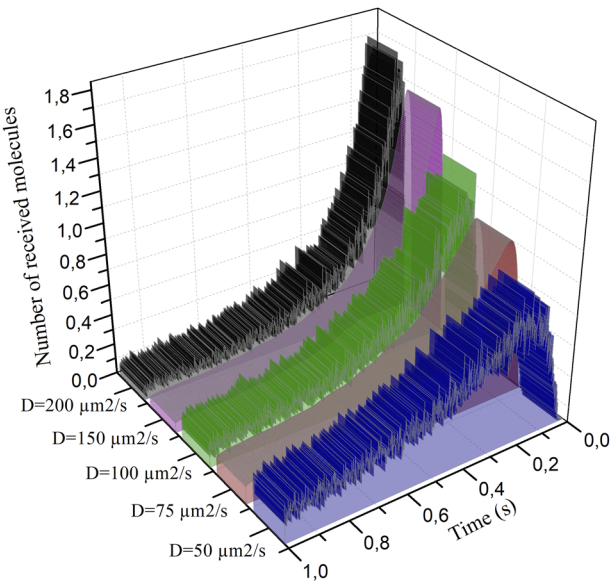

FIG. 9. Number of received molecules versus time using D values of 50, 100, and 200 $\mu m^2/s$ for simulation results and D values of 75 and 150 $\mu m^2/s$ for predicted results of a fixed system with the ANN.

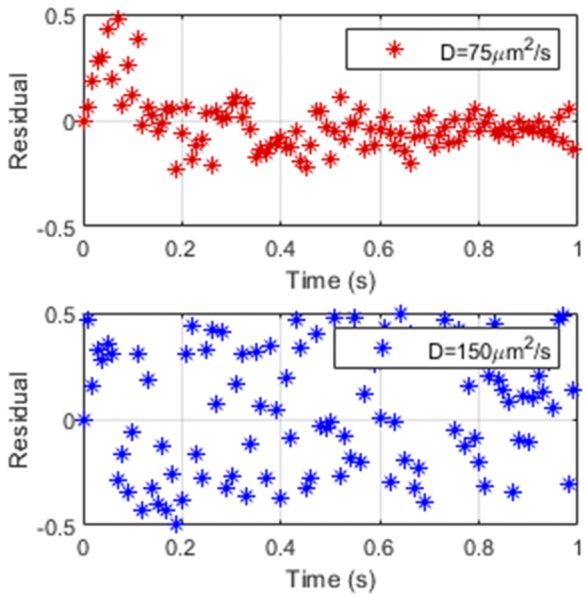

FIG. 10. Residual values between predicted and simulation results of a mobile system for D values of 75 and 150 $\mu m^2/s$.

results of the model, MSE values are obtained at almost 0 especially for the testing part of the model.

As shown in Figs. 8 and 9, the number of received molecules was simulated for diffusion constants of 50, 100, and 200 $\mu m^2/s$ by using the proposed NSS model, and it is predicted by using the ANN for values of 75 and 150 $\mu m^2/s$. The difference between simulation and predicted values is obtained using the residual method with respect to the number of received molecules as shown in Figs. 10 and 11 for mobile and fixed system models. These results show us that the accuracy is promising for prediction of mobile and fixed system models. As indicated in Figs. 10 and 11, the residual

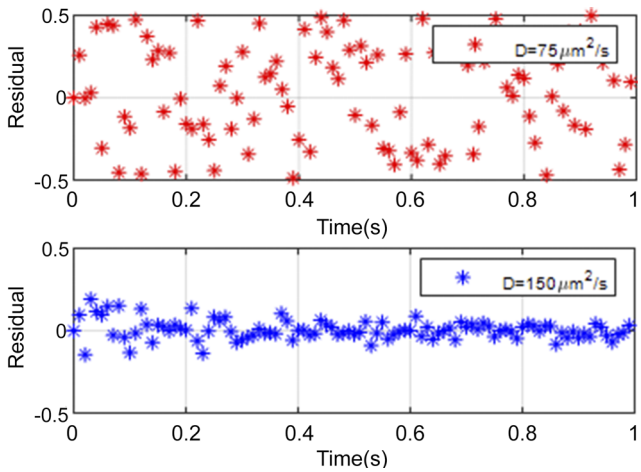

FIG. 11. Residual values between predicted and simulation results of fixed system for D values of 75 and 150 $\mu m^2/s$.

values are obtained with a very small range between +0.5 and −0.5 for both system models. For the mobile system, as the mobility was higher than the fixed system, the number of received molecules was more. This is due to the mean free path of the moving molecules being longer while diffusing for the mobile system.

IV. CONCLUSION AND FUTURE WORK

In this paper, we have proposed a new NSS model, which has a spherical shape, of the receiver to increase hitting probability. As far as the author knows, there is no such comprehensive study for the mobile and fixed systems by comparing and predicting diffusion constant using the ANN in the literature. For the mobile system, as the mobility was higher than the fixed system, the number of received molecules was more. The diffusion constant of the medium was also predicted by using an artificial neural network and compared with the simulation results with respect to the residual analysis. As a result of the analysis, it is predicted by using the ANN for the diffusion constants of 75 and 150 $\mu m^2/s$ with a small range of residual values of ±0.5 for both of the mobile and fixed systems. These results showed that the ANN can be used in such systems in the future studies.

AUTHOR DECLARATIONS

Conflict of Interest

The author declares that they have no conflict of interest.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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