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Effect of Diffusion Constant on the Interference and Probability of Molecule Reception in MCvD

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Abstract— Many study have been conducted highly regarding for Molecular Communication via Diffusion (MCvD) to contribute to the developments in the field of nano-technology. In this study, a new MC model by using the point transmitter and spherical receiver that can be used in nano-scale systems was developed and analyzed in terms of communication performance using the Monte Carlo simulations. The carrier particles that is used to convey information between transmitter and receiver consist of biological components such as DNA and protein components. The proposed MC model that can possibly be used in nano-scale systems is analyzed in terms of channel performance of communication such as diffusion constant. The number of received molecules and signal to interference ratio (SIR) are analyzed by using physical definition of the Fick's second low. Finally it is obtained that the probability of a molecule reception of the receiver and SIR value increase with increasing Diffusion constant for the proposed MC model.

Keywords : *Diffusion constant, interference, molecular communication.*

1. Introduction

Many study have been carried out about communication of nano-devices in recent years (Akyildiz, Brunetti, & Blázquez, 2008; Farsad, Yilmaz, Eckford, Chae, & Guo, 2014; Nakano, Tadashi, ANDREW W. ECKFORD, 2013). The transmitter (Tx) and receiver (Rx) parts are investigated to analyze transmitted and received molecules in a fluid media (Isik, I., Yilmaz, H. B., Demirkol, I., & Tagluk, 2020). However, generally the Rx entity and the received signal are considered to analyze MC systems. In (Yilmaz, Heren, & Tugcu, 2014), channel transfer function by using a fully absorbing spherical receiver and point transmitter for molecular communication via diffusion (MCvD) is presented with analytic and simulation studies. In this study, in a 3-dimensional (3-D) environment, propagation delay and attenuation are studied for channel of MCvD model. Pulse amplitude and pulse peak time are investigated regarding distance between receiver and transmitter. Finally it is found that when the distance and pulse peak time increased then pulse amplitude decreased. Moreover molecular antenna models for MCvD are also studied in literature.

In MC, chemical transceiver models can be used for the implementation subjects to send information from transmitter to receiver. It is known that this models can be applied to many fields such as defense, environmental monitoring, bio-medical, industrial and dentistry purposes (Akkaya, Yilmaz, Chae, & Tugcu, 2015; Akyildiz et al., 2008; Farsad et al., 2014; Nakano, Tadashi, ANDREW W. ECKFORD, 2013; Yilmaz et al., 2014). In this studies, because of their parallel structure to the digital antennas usually receptors have been considered as the molecular antenna. It is known that all biological cells have receptors which is placed at the surface of their receiver to receive nutrient, proteins or other substances (Işik, Er, & Tağluk, 2020). In (Akkaya et al., 2015), the hitting probability of MCvD system for a point transmitter and spherical receiver is analyzed by changing the parameters of density and size of these receptors. The absorption rate of receiver is also analyzed analytically by using hitting probability versus the number and the size of receptors. It is concluded from (Akkaya et al., 2015) that deployment of small receptors on the receiver instead of larger receptor, the hitting probability is obtained higher when the total receptor deployment area remains the same. The minimum sufficient surface area of receptor is also investigated in this study and finally it is found that displacement of the receptors on the receiver should be as little as 1% of the surface area of the receiver to have a comparable signal energy with a perfectly absorbing spherical receiver.

Einolghozati et al. have proposed a receiver with ligand receptors (Einolghozati, Sardari, & Fekri, 2011), which include bins for molecules to interpose and start signaling inside the cell. In this pioneering study, the receiver of the system has been considered to possess a large number of binding seats and the molecular concentration over each of these seats has been calculated with a Markov Chain model. The total reception ratio of a receiver has been estimated by averaging the concentrations over all binding seats (Einolghozati et al., 2011). In order to test the system for achieving higher reception ratios, the transmitter released molecules at either low or high concentrations to achieve "low" and "high" signal levels similar to binary generators. As a result, authors are obtained the capacity of ligand receptor, which was increased for a higher number of receptors. In such models, medium ratio of concentrations are avoided at the transmitter side to not to cause any ambiguity as neither "low" nor "high". CNTs (carbon nanotubes) and GNRs (Graphene Nanoribbon) based molecular receptor antenna models using graphane and its derivatives are also analyzed due to their prominent sensing capabilities in nano sensor networks (Farsad et al., 2014). In another model (Singh & Singh, 2016), a molecular antenna model is proposed and some coding techniques are introduced for the proposed system.

To increase the ratio of reception, a novel architecture of antenna models, which are mainly composed of a spherical receiver and supported with a totally reflective spherical or cylindrical shell oriented over or around the receiver, has been introduced in (Felicetti, Femminella, & Reali, 2018). Different shape of a shell such as sphere and cylinder which is placed on the receiver is considered as antenna and numbers of absorbed molecules are increased with these shells.

In (Isik, 2020), a novel architecture of receiver model by using different channel environment parameter such as diffusion constant which can be used for receiving part of MC systems for MCvD is introduced. In our study, we propose the use of different value of diffusion constant in the environment instead of the same value of it used in the literature. Through Monte Carlo simulations we evaluate the effect of diffusion constant on the reception ratio, which suggests better channel parameter possibilities in terms of reception probability.

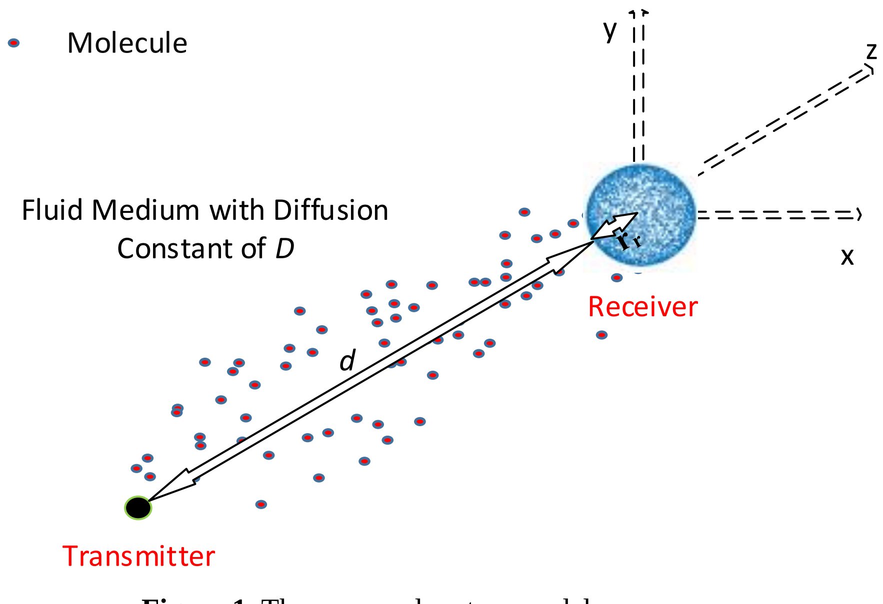

Figure 1. The proposed system model.

2. Material and Methods

In the study, the physical properties of the channel of MCvD model are examined using point transmitter and spherical transmitter. It is known that the transfer of information between the receiver and the transmitter takes place by carriers such as molecules in the environment. The physical properties of the carriers and the density of the medium are very important for the information transfer.

The number of current density, which can be an atom, hole, electron, and molecule, determines the current, which is the charge flow rate. Since it is known as the number of charge carriers, the current flowing can also be calculated. There are two current flow mechanisms that cause charges to move, drift and diffusion. Charge moves under the influence of an electric field since the applied field exerts a force (Walter & Vreeburg, 1989),

$$F = m^* \frac{dv}{dt} = qE, \quad (1)$$

In the following, q denotes a general charge; also consider an isotropic effective mass m^* at first. After E represents applied field and F represents force. This movement results a current which is known as drift current,

$$I_d = nqV_dA, \quad (2)$$

where I_d, V_d, A, n and q are drift current, drift velocity of charge carrier, area of the medium, number of charge carriers per unit volume, charge of electron respectively. Carrier mobility, μ is a measure how easily charge carriers move under the influence of an applied field or μ determines how mobile the charge carriers are (Walter & Vreeburg, 1989),

$$V_d = \mu E. \quad (3)$$

If the medium is at thermodynamic equilibrium (there is no applied field) the carrier have a thermal energy of $\frac{k_B T}{2}$ per degree of freedom and in 3D the thermal energy of electron,

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

where V_{th}, k_B, m* and T refer to thermal velocity of electron, Boltzman Constant ($1.38 * 10^{-23}$ J/K), the 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 result no net current flow. Molecules move in the system due to its thermal energy or applied field but they collide each other. The average time taken between collisions is called as relaxation time or mean free time, τ. So we can define the mobility as,

$$\mu = \frac{q\tau}{m^*}. \quad (5)$$

Diffusion current is due to the movement of the carriers from high concentration region towards to low concentration region. As the carriers diffuse, a diffusion current flows. The force behind the diffusion current is the random thermal motion of carriers. A concentration gradient produces a pressure gradient which produces the force pressure gradient which produces the force on the molecules causing to move them (Walter & Vreeburg, 1989). According to electrical mobility equation, diffusion constant for charged particles is defined as follow,

$$D = \frac{\mu k_B T}{q} . \quad (6)$$

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 transmission medium is determined with diffusion coefficient; D for diffusion of spherical uncharged particles through a liquid is given,

$$D = \frac{k_B T}{\zeta}, \tag{7}$$

where ζ drag coefficient and it is defined as follow,

$$\zeta = 6\pi\eta R_H, \tag{8}$$

where R_H refer to the hydraulic radius of the information particle. The number of hitting molecules until time *t*, N_{hit}^{1D}(t) is given below,

$$N_{hit}^{1D}(t) = erfc(\frac{d}{\sqrt{4Dt}}), \tag{9}$$

where *erfc* and *d* refer error function and distance between transmitter and receiver respectively. In an MC system, the number of received molecules in the first symbol duration to the number of transmitted molecules, in other words, the ratio of received molecules in the duration of first symbol slot is given as follow,

$$h_0 = \frac{N_{rx}(0)}{N_{tx}(0)}, \tag{10}$$

where $\mathrm{N_{rx}}(0)$ and $\mathrm{N_{tx}}(0)$ refer to total number of molecules received by the receiver and total number of molecules released from the transmitter during the first symbol duration. *SIR* (signal to interference rate), which is known as (ISI) inter-symbol-interference in literature, is equal to ratio of probability of the received molecules in the first symbol duration and probability of the received molecules after the first symbol duration

$$SIR = \frac{h_0}{\sum_{k\in(1,\ldots.son)} h_k} \tag{11}$$

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

3. Results

In this study, the proposed MC model is analyzed by changing the diffusion constant of the medium. System parameters of the proposed model are given in Table 1. Effect of diffusion constant on receiver models are analyzed by using hitting probability of received molecules and signal to interference rate which are h_0 and *SIR* metrics. h_0 is probability of hitting molecules in first t_s (symbol duration) and SIR is interference after the first symbol duration. In this study, shape of transmitter is chosen as a point source and shape of receiver is chosen as spherical. In this view, firstly we analyze sphere receiver model for different diffusion constant values which are 40, 60, 79 and 100 $\mu m^2/s$ to obtain the best MC model. As shown in Fig. 1 the highest number of molecules is found highest for D=100 $\mu m^2/s$ and the value of *SIR* is also found highest for *D*=100 $\mu m^2/s$. It is concluded that, probability of received molecules in the receiver increase with increasing diffusion constant of the fluid. Since an environment with a high diffusion coefficient or low viscosity would have little effect on the spreading rate of the molecules in the medium. Viscosity has a reverse relationship with diffusion constant as given in Eq. 7. The proposed model is also analyzed for *SIR* value in Fig. 2. As seen from the figure, when the diffusion constant decrease, *SIR* value also decrease as expected. Since value of the viscosity increased, the spreading rate of the molecules in the medium decreased as shown in Eq. 7 and 8.

Table 1. System parameters

r_r, radius of the receiver	3.101 μm^3
d, distance between receiver and transmitter	5 μm
r_s, radius of receptor	0.04 μm
Number of receptor	5000
Number of transmitted molecules	20000
D, diffusion constant	40, 60, 79.4, 100 $\mu m^2/s$
R_H	2.86 nm
T	310 K
Number of simulations	100

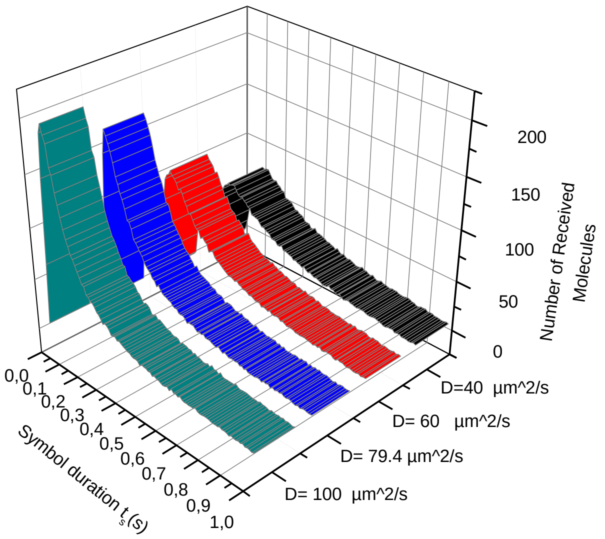

Figure 1. Number of received molecules versus symbol duration graph with changing of *D*

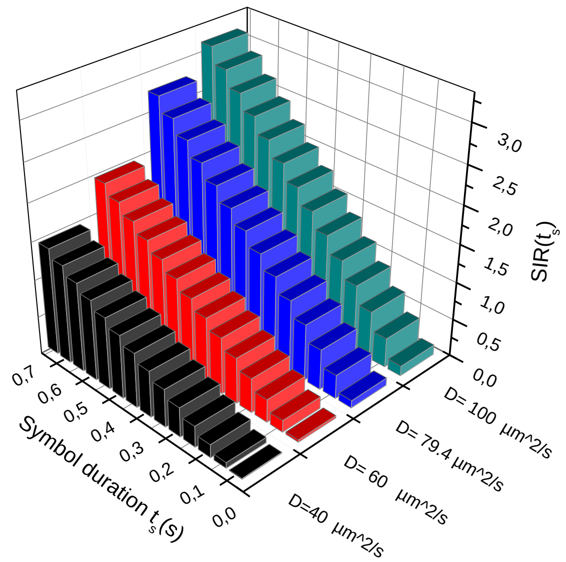

Figure 2. *SIR* versus symbol duration graph with changing of *D*

4. Conclusion

In this study, the number and reception ratio of the received molecules are analyzed by changing the diffusion coefficient in the environment. Software based MCvD model is developed with point transmitter and spherical receiver. It was observed that when the viscosity of diffusion coefficient increase the number and probability of receiving molecule decrease. Due to the collision of molecules, carriers may be move slowly or lost their energy to move. Therefore when the symbol duration increased, the number of received molecules decreased. According to the Fig. 1 we observed that the relaxation time of molecules is about 0.1 s as shown in Fig. 1. Because after 0.1 s, the number of received molecules decreased sharply. As a result, the diffusion coefficient of the medium can be changed in order to increase information transfer with lower error.

As a future work, we plan to find new antenna models to increase hitting probability and to decrease effect of environment on diffusion of molecules.

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