

# An Information Theoretical Approach for Molecular Communication

(Invited Paper)

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## ABSTRACT

Molecular communication is a novel communication paradigm which allows nanomachines to communicate using molecules as a carrier. Controlled molecule delivery between two nanomachines is one of the most important challenges which must be addressed to enable the molecular communication. Therefore, it is essential to develop an information theoretical approach to find out molecule delivery capacity of the molecular channel. In this paper, we develop an information theoretical approach for capacity of a molecular channel between two nanomachines. We first introduce a molecular communication model. Then, using the principles of mass action kinetics we give a molecule delivery model for the molecular communication between two nanomachines called as Transmitter Nanomachine (TN) and Receiver Nanomachine (RN). Then, we derive a closed form expression for capacity of the channel between TN and RN. Numerical results show that selecting appropriate molecular communication parameters such as temperature of environment, concentration of emitted molecules, distance between nanomachines and duration of molecule emission, it can be possible to achieve maximum capacity for the molecular communication channel between two nanomachines.

## Keywords

Molecular communication, information theory, channel capacity, entropy.

## 1. INTRODUCTION

Molecular Communication is a new interdisciplinary research area including the nanotechnology, biotechnology, and communication technology [1]. In nature, molecular communication is one of the most important biological function in

living organisms to enable biological phenomena to communicate with each other. For example, in an insect colony, insects communicate with each other by means of pheromone molecules. When an insect emits the pheromone molecules, some of them bind the receptors of some insects in the colony and these insects convert the bound pheromone molecules to biologically meaningful information. This enables the insects in the colony to communicate with each other. Similar to insects, almost all of the biological systems in nature perform intra-cellular communication through vesicle transport, inter-cellular communication through neurotransmitters, and inter-organ communication through hormones [1].

Nanotechnology is one of the most important promising technology which enables nano-scale machines called as nanomachines [2]. Nanomachines are molecular scale objects that are capable of performing simple tasks such as actuation and sensing [1]. Nanomachines are categorized into two types [2]. While one type mimics the existing machines, other type mimics nature made nanomachines such as molecular motors and receptors [2]. In the biological systems, communication among the cells forming the biological system is essential to enable the cells to effectively accomplish their tasks. For example, in natural immune system, the white blood cells called as B-cells and T-cells communicate with each other to eliminate the pathogen entering the body. Similar to biological systems, communication among nanomachines is essential for effective sensing and action.

Since nanomachines are limited in their size and capabilities, the traditional wireless communication based on electromagnetic waves cannot be possible to communicate two nanomachines [1]. However, instead, the molecular communication is a viable communication paradigm which allows the nanomachines to communicate with each other using molecules as information carrier [1]. Therefore, it is essential to find out molecule delivery capacity of a molecular channel between two nanomachines based on molecular communication parameters such as temperature of environment, concentration of emitted molecules, distance between nanomachines and duration of molecule emission.

There exist several research efforts about the molecular communication in the literature. In [1], research challenges in molecular communication is manifested. In [3], the concept of molecular communication is introduced and first attempt for design of molecular communication system is per-

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formed. In [4], a molecular motor communication system for molecular communication is introduced. In [5], a molecular communication system which will enable future health care applications is investigated. In [6], based on intercellular calcium signaling networks, the design of a molecular communication system is introduced. In [7], an autonomous molecular propagation system is proposed to transport information molecules using DNA hybridization and biomolecular linear motors. The existing studies about the molecular communication include feasibility of the molecular communication and design schemes for molecular communication system. However, none of these studies investigate the capacity of a molecular channel to understand possible conditions in which the molecular communication can be feasible and high molecular communication capacity can be achieved.

In this paper, we introduce an information theoretical approach for molecular communication system. Using the principles of mass action kinetics, we first model the molecular delivery between two nanomachines called Transmitter Nanomachine (TN) and Receiver Nanomachine (RN). Then, based on the molecular delivery model, we derive the closed form expression for capacity of the channel between TN and RN. According to the capacity expression, we investigate how the conditions such as temperature of environment, concentration of emitted molecules, distance between nanomachines and duration of molecule emission affect the molecular communication capacity. Then, we discuss under which conditions the molecular communication can be feasible and can achieve which capacity.

The remainder of this paper is organized as follows. In Section 2, we introduce a molecular communication model. In Section 3, we introduce a molecule delivery approach for the molecular communication between two nanomachines. In Section 4, based on the molecule delivery scheme we introduce an information theoretical approach for the molecular communication between two nanomachines. In Section 5, we evaluate the numerical results over the given approach and we give concluding results in Section 6.

## 2. MOLECULAR COMMUNICATION MODEL

Nanomachines are categorized into two types [2]. First type is the nanomachines which mimic the existing machines. Second type is the nanomachines analogous to the existing biological mechanism such as cells and cell components. In this paper, we consider a kind of nanomachine which is analogous to the biological mechanisms. In nature, molecular communication between biological mechanisms is based on the ligand-receptor binding mechanism. According to ligand-receptor binding mechanism, ligand molecules are emitted by one biological phenomenon then, the emitted ligand molecules diffuse in the environment and bind the receptors of another biological phenomenon. This binding enables the biological phenomenon to receive the bound molecules by means of the diffusion on cell membrane. The received ligand molecules allow the biological phenomenon to understand the biological information. For example, in biological endocrine system, gland cells emit hormones to inter-cellular environment then, hormone molecules diffuse and are received by corresponding cells. According to the type of emitted hormone, the corresponding cells convert the hormone molecule to biologically meaningful information. This natural mechanism provides the molecular communication for almost all biological phenomena.

In this paper, we adopt this natural ligand-receptor binding mechanism to enable the molecular communication between nanomachines called Transmitter Nanomachine (TN) and Receiver Nanomachine (RN) as shown in Fig. 1. In the literature, artificial ligand-receptor binding schemes have been previously introduced [8], [9]. In this paper, we use an artificial ligand-receptor binding model developed in [8]. We assume that TN is a nano-scale machine or a biological entity and it can emit one kind of molecule called  $A$ . We also assume that TN emits molecules  $A$  with concentration  $L(t)$  according to the following emission pattern [9] which is similar to alternating square pulse.

$$L(t) = \begin{cases} L_{ex} & \text{for } jt_H \leq t \leq jt_H + t_H \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

where  $j = (0, 1, \dots)$ ,  $t_H$  is the duration of the pulses and  $L_{ex}$  is concentration of molecules  $A$  emitted by TN. Furthermore, we assume that RN is a nano-scale machine and it has  $N$  receptors called  $R$  on its surface. The receptors enable RN to receive the molecules which bind their surface.

In traditional digital communication, information sequences are transmitted via two bits, logic 1 and 0. If a transmitter detects a voltage level which is greater than a prescribed voltage level in the channel, it decides that transmitter transmitted logic 1. If the voltage level in the channel is less than the prescribed level, the receiver decides that the transmitter transmitted logic 0. Using this traditional idea, we propose a similar molecular communication scheme. According to this scheme, during time interval  $t_H$  TN can emit either molecules  $A$  corresponding to logic 1 in digital communication or it transmits no molecule corresponding to logic 0 in digital communication. If a TN intends to transmit molecules  $A$ , we assume that during the time interval  $t_H$ , it emits molecules  $A$  to its surrounding environment with a specific concentration  $L_{ex}$ . Similar to logic 1 and logic 0 in traditional digital communication, we denote the case that TN transmits molecules  $A$  with  $A$  and we denote the case that TN transmits no molecule with 0. Hence, for the molecular communication model, we have two molecular communication bits called  $A$  and 0.

At RN side, these bits are inferred via concentration of molecules  $A$  such that if an RN can receive a concentration of molecules  $A$  which is greater than a prescribed concentration called as  $S$  ( $\mu\text{mol/liter}$ ), the RN decides that the TN transmitted molecular bit  $A$  during the time interval  $t_H$ . Conversely, if the RN can receive a concentration of molecules  $A$  which is less than  $S$ , the RN decides that the TN transmitted molecular bit 0.

In traditional digital communication, noise level in the channel causes the channel errors such that when a transmitter intends to transmit logic 0, the receiver may detect logic 1, or for logic 1, the receiver may detect logic 0 due to the noise in the channel. Similarly, in the molecular communication, it may be possible to detect erroneous molecular communication bits at the RN side. During the molecular communication, the molecules  $A$  are emitted by TN and the emitted molecules continuously diffuse to surrounding environment including the RN such that molecules  $A$  always exist and diffuse in the environment. Therefore, due to the emitted molecules  $A$  which diffuse in the surrounding environment, it is possible for RN to receive molecular bit  $A$  although TN transmits molecular bit 0. Furthermore, due to delay in diffusion of molecules  $A$  to RN it is also possible

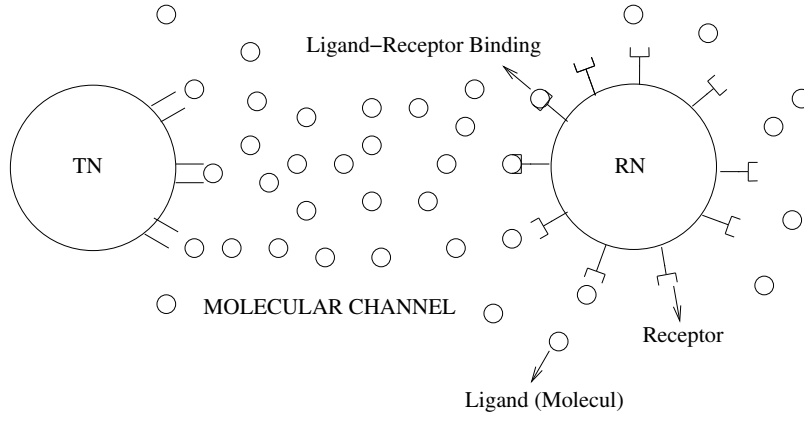


Figure 1: Molecular Communication Model.

for RN to receive molecular bit 0 although TN transmits molecular bit  $A$ . Moreover, erroneous molecular bits can arise some factors which affect the molecular diffusion between TN and RN, such as temperature of the environment, concentration of emitted molecules  $A$ , distance between TN and RN, duration of molecule emission, binding and release rates and number of receptors on RN.

Thus, similar to traditional digital communication channel, the molecular communication channel between TN and RN has a molecule delivery capacity which is defined as maximum number of non-erroneous molecular bits which can be delivered within a specific time duration.

Next, we introduce a molecule delivery model for the molecular communication between TN and RN according to the molecular communication model given above.

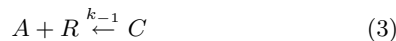
### 3. MOLECULE DELIVERY

For the molecular communication between TN and RN, it is important to understand how molecules  $A$  can be delivered to RN by means of the binding between molecules  $A$  and receptors  $R$  on the RN. In this section, following the ligand-receptor binding model introduced in [8], we introduce a model for the molecule delivery from TN to RN.

According to the ligand-receptor binding reaction kinetic, when molecules  $A$ , emitted by TN, encounter with receptors  $R$  on RN, molecules  $A$  bind the receptors  $R$ . These bound molecules  $A$  and receptors  $R$  constitute complexes  $C$  (bound receptors) according to the following chemical reaction,



where  $k_1$  ( $\mu\text{mol/liter/sec.}$ ) is rate of binding reaction. Similar to the binding reaction, it is possible to release molecules  $A$  from receptors  $R$  according to the following chemical reaction,



where  $k_{-1}$  ( $1/\text{sec.}$ ) is rate of release reaction.

As given in (1), TN emits molecules  $A$  via a square pulse with amplitude  $L_{ex}$  during  $t_H$  ( $\text{sec.}$ ). In this duration, concentration of bound receptors  $C(t)$  ( $\mu\text{mol/liter}$ ) can be given [8] as follows

$$C(t) = C_\infty(1 - e^{-t(k_{-1} + k_1 L_{ex})}) \quad (4)$$

where  $k_1$  and  $k_{-1}$  are the binding and release rates, respectively,  $L_{ex}$  ( $\mu\text{mol/liter}$ ) is concentration of molecules  $A$  which is emitted by TN.  $C_\infty$  is steady state level of bound receptors and can be given [8] as follows

$$C_\infty = \frac{k_1 L_{ex} N}{k_{-1} + k_1 L_{ex}} \quad (5)$$

where  $N$  ( $\mu\text{mol/liter}$ ) is the concentration of receptors ( $R$ ) on RN.

During the pulse duration  $t_H$ ,  $C(t)$  rises exponentially according to (4) [8]. At time  $t_0$  when the pulse duration ends,  $C(t)$  starts to decay [8] according to

$$C(t) = C_{t_0} e^{-(k_{-1}(t-t_0))} \text{ for } t > t_0 \quad (6)$$

The rates of molecule/receptor interaction,  $k_1$  and  $k_{-1}$ , can depend on molecular diffusion from TN to RN. More specifically, while the binding rate  $k_1$  heavily depends on the molecular diffusion parameters from TN to RN such as diffusion coefficient, temperature of environment, distance between TN and RN [11], the release rate  $k_{-1}$  depends on some environmental factors such as interaction range and temperature [12]. Here, we do not predict  $k_1$  according to the diffusion parameters of the environment. In fact, binding rate  $k_1$  can be captured with analytical expressions [15]. However, this is out of scope of this paper. Here, we only assume that binding rate ( $k_1$ ) is inversely proportional with distance ( $\alpha$ ) between TN and RN such that  $k_1 \propto 1/\alpha$  and it is directly proportional with temperature of environment ( $T$ ) such that  $k_1 \propto 2T$ . For the release rate  $k_{-1}$ , we use the model given in [12] as follows

$$k_{-1} = k_{-1}^0 e^{\alpha f / k_B T} \quad (7)$$

where  $k_{-1}^0$  is the zero-force release rate,  $\alpha$  is the distance between TN and RN,  $k_B$  and  $T$  are the Boltzmann constant and absolute temperature, respectively.  $f$  is the applied force per bound.  $f$  is related with the energy of the emitted molecules and the distance between TN and RN and the environmental factors [14]. Here, we consider  $f$  as positive constant throughout this paper.  $k_{-1}^0$  can be predicted by

fitting the experimental measurements [12] and it is related with the capability of molecule capturing of RN receptors. Therefore, we assume that  $k_{-1}^0$  is a variable which depends only on properties of RN receptors.

Based on the models introduced in Section 2 and 3, we next introduce an information theoretical approach for capacity of the molecular channel between TN and RN. According to total concentration of complex molecules ( $C(t)$ ) forming in RN and expressed in (4), (5) and (6), we derive probability of erroneous molecular bits which cannot successfully delivered to RN and we can give capacity of the molecular channel between TN and RN.

#### 4. AN INFORMATION THEORETICAL APPROACH FOR MOLECULAR COMMUNICATION

As introduced in Section 2, for the molecular communication between TN and RN, two molecular bits are available. Every time when TN transmits a molecular bit, concentration of delivered molecules determines success of the transmission. If TN transmits molecular bit  $A$ , at least  $S$  number of molecules<sup>1</sup>  $A$  must be delivered to RN within time interval  $t_H$  for a successful delivery of a molecular bit  $A$ . If TN transmits molecular bit 0, number of molecules  $A$  delivered within  $t_H$  must be less than  $S$  for a successful delivery of molecular bit 0. Therefore, it is imperative to find number of delivered molecules in each transmission interval  $t_H$  to determine the success of the molecular bit transmission from TN to RN. Here, using (4), (5), (6) and (7), we find the close form expressions for expected value of number of delivered molecules  $A$  during  $t_H$ .

For the case that TN emits molecules  $A$  during  $t_H$ , number of delivered molecules  $A$  within  $t_H$ , i.e.,  $N_A$ , can be given by integrating (4) from 0 to  $t_H$  as follows

$$N_A = \int_0^{t_H} C(t)dt \quad (8)$$

$$N_A = \int_0^{t_H} \frac{k_1 L_{ex} N}{k_{-1} + k_1 L_{ex}} (1 - e^{-t(k_{-1} + k_1 L_{ex})}) dt \quad (9)$$

Since the molecular diffusion continues after every  $t_H$  interval, the previous molecular bits affect the number of delivered molecules  $A$  in current interval. Therefore, the number of delivered molecules  $A$  in current interval also depends on molecular bits transmitted in the previous intervals according to exponential decay in number of complex as introduced in (6). Here, we assume that last molecular bit only affects the current molecular transmission since number of delivered molecules exponentially decay after time  $t_H$  according to (6). If we assume that TN emits  $A$  molecules with probability  $P_A$  in each time interval  $t_H$  and it emits molecular 0 bit with probability  $(1 - P_A)$ . Hence, the effect of the last emitted molecular bit to current molecular bit transmission can be considered as expected number of complexes coming from the previous interval, i.e.,  $N_p$ . Thus, using (6),  $N_p$  can be given as follows

<sup>1</sup>Since concentration of molecules ( $\mu\text{mol/liter}$ ) can be converted to number of molecules by multiplying Avagadro constant ( $6.02 \times 10^{23}$ ), here we use sometimes number of molecules instead of concentration of molecules.

$$N_p = \int_0^{t_H} \left( P_A \int_0^{t_H} C(t)dt \right) e^{-(k_{-1}t)} dt \quad (10)$$

$$N_p = \int_0^{t_H} \left( P_A \int_0^{t_H} \frac{k_1 L_{ex} N}{k_{-1} + k_1 L_{ex}} (1 - e^{-t(k_{-1} + k_1 L_{ex})}) dt \right) e^{-(k_{-1}t)} dt \quad (11)$$

Combining (9) and (11), for the case that TN emits  $A$  molecules during  $t_H$ , expected value of total number of delivered molecules  $A$ , i.e.,  $E[N_{TA}]$ , can be given as follows

$$E[N_{TA}] = N_A + N_p \quad (12)$$

At the RN side, if RN can receive  $S$  number of molecules  $A$ , it infers that TN emitted the molecular bit  $A$  during  $t_H$ . Thus, using the well-known Markov inequality, we can give a maximum bound for the probability  $p_1$  that TN achieves to deliver molecular bit  $A$  as follows

$$p_1(N_{TA} \geq S) \leq \frac{E[N_{TA}]}{S} \quad (13)$$

Hence, TN achieves to deliver molecular bit  $A$  with maximum probability  $p_1 = \frac{E[N_{TA}]}{S}$  and RN receives molecular bit 0 instead of the molecular bit  $A$  such that TN does not succeed to deliver  $A$  with probability  $(1 - p_1)$ .

For the transmission of molecular bit 0 during  $t_H$ , the number of delivered molecules  $A$  only depends on lastly emitted molecular bit since TN transmits no molecules during the transmission of molecular bit 0. Therefore, following (11), we can give expected value of total number of delivered molecules  $A$  within  $t_H$  for the transmission of molecular bit 0, i.e.,  $E[N_{T0}]$ , as follows,

$$E[N_{T0}] = N_p \quad (14)$$

For the transmission of molecular bit 0, using the Markov inequality, we can give the following maximum bound for the probability  $p_2$  that TN achieves to deliver molecular bit 0 such that RN receives a number of molecules  $A$  which is less than  $S$  and ( $N_{T0} \leq S$ ).

$$p_2(N_{T0} \leq S) \leq \frac{S}{E[N_{T0}]} \quad (15)$$

Hence, for the transmission of molecular bit 0, TN achieves to deliver molecular bit 0 with maximum probability  $p_2 = \frac{S}{E[N_{T0}]}$  and it does not achieve to deliver molecular bit 0, instead, it incorrectly delivers molecular bit  $A$  with probability  $(1 - p_2)$ .

According to the transmission probabilities  $p_1$  and  $p_2$ , we can model a channel similar to the symmetric channel. If we consider that TN emits molecular bit  $X$  and RN receives molecular bit  $Y$ , then the transition matrix of the molecular channel can be given as follows

$$P(Y/X) = \begin{pmatrix} P_A p_1 & P_A (1 - p_1) \\ (1 - P_A) p_2 & (1 - P_A) (1 - p_2) \end{pmatrix}$$

Based on the transition matrix  $P(Y/X)$ , we can give the mutual information  $I(X; Y)$  between  $X$  and  $Y$  which states number of distinguishable molecular bits, i.e,  $M$  as follows

$$M = (H(P_A p_1 + (1 - P_A)(1 - p_2), P_A(1 - p_1) + (1 - P_A)p_2) - (P_A H(p_1, 1 - p_1) + (1 - P_A) H(p_2, 1 - p_2))) \quad (16)$$

where  $H(\cdot)$  denotes the entropy. We also give  $M$  in (18). According to  $M$ , we can give the capacity of molecular channel between TN and RN i.e.,  $C_M$  as follows

$$C_M = \max(M) \quad (17)$$

Next, we give the numerical results over the capacity of molecular communication channel given in (16).

## 5. NUMERICAL RESULTS

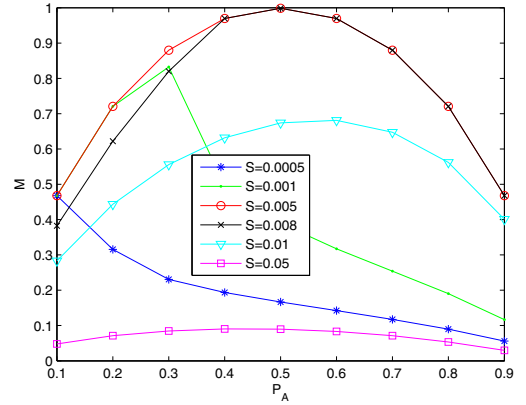
In this section, we give the numerical results performed over the expression given in (18). We perform the numerical analysis using Matlab. For this analysis, we assume that two nanomachines called as TN and RN are positioned in an environment which may have different diffusion coefficients for each analysis such that it allows TN to achieve different binding rates ( $k_1$ ). Furthermore, we assume that  $k_1$  is a variable changing with temperature of environment ( $T$ ) and distance ( $\alpha$ ) between TN and RN such that  $k_1 \propto 2T$  and  $k_1 \propto 1/\alpha$ , respectively. Moreover, we assume that  $k_{-1}^0$  depends only on the properties of RN receptors and can be changed. We give the simulation parameters of this analysis in Table 1.

**Table 1: Simulation Parameters**

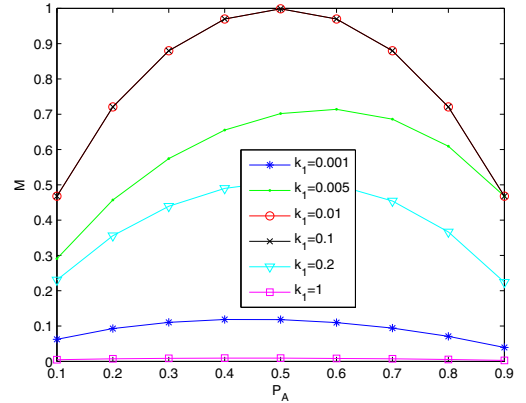
Binding rate ( $k_1$ )	0.001-1 ( $\mu\text{mol/liter/s}$ )
Zero-force release rate ( $k_{-1}^0$ )	0.001-0.1 ( $\text{s}^{-1}$ )
Temperature ( $T$ )	300-1000 K
Distance between TN and RN ( $\alpha$ )	$5^{-10} - 4 \times 10^{-9} \text{m}$
Applied force per bound ( $f$ )	$10^{-12}$ (J/m)
Concentration of molecules A ( $L_{ex}$ )	0.05-1.5 ( $\mu\text{mol/liter/s}$ )
Duration of the pulses ( $t_H$ )	0.1-1 s
Number of receptors $R$ ( $N$ )	0.0001-0.005 ( $\mu\text{mol/liter}$ )
$S$	0.0005-0.05 ( $\mu\text{mol/liter/s}$ )

For the first analysis in Fig. 2,  $M$  is shown with varying  $P_A$  for different  $S$ . For  $S = 0.0005 - 0.001$ ,  $M$  and maximum value of  $M$  ( $C_M$ ) are very small because erroneous molecular bits arise when molecular bit 0 is transmitted. For this analysis,  $k_1 = 0.05$  is used. Since  $S$  is much smaller than  $k_1$ , TN cannot achieve a concentration smaller than  $S$  for the transmission of molecular bit 0 such that the transmission of molecular bit 0 causes the delivery of molecular bit A and error occurs. Therefore,  $M$  and  $C_M$  are small for  $S = 0.0005 - 0.001$ . However, for  $S = 0.005 - 0.008$ ,  $M$  and  $C_M$  can be increased and maximized using the appropriate  $P_A$  since it can be possible to deliver non-erroneous molecular bits. In this case, since  $S$  is sufficiently high with respect to  $k_1 = 0.05$ , erroneous molecular bits do not arise in transmission of molecular bit 0. For  $S = 0.008 - 0.05$ ,  $M$  and  $C_M$  again start to decrease. The reason for this is that for higher values of  $S$ , it cannot be possible to deliver a concentration higher than  $S$  for transmission of molecular bit A. This causes erroneous delivery of molecular bit A and  $M$  and  $C_M$  again decrease. As a result, we can say that for  $S$  which is near  $k_1$ , the capacity of molecular channel is very low. Therefore, it is necessary to select appropriate  $S$  smaller than  $k_1$  to maximize  $M$  and  $C_M$ .

In Fig. 3,  $M$  is shown with varying  $P_A$  for different  $k_1$ . In this analysis,  $S = 0.005$  is used. For the  $k_1$  which is near the  $S$  (0.001-0.005),  $M$  and  $C_M$  are very small. In this case,



**Figure 2:  $M$  with varying  $P_A$  for different  $S$ .**



**Figure 3:  $M$  with varying  $P_A$  for different  $k_1$ .**

since  $k_1$  is very small, the needed concentration  $S$  cannot be delivered for successful delivery of molecular bit A and,  $M$  and  $C_M$  decrease. For  $k_1 = 0.01 - 0.1$ , sufficient concentration higher than  $S$  for molecular bit A can be delivered and,  $M$  and  $C_M$  increase. However, while  $k_1$  is further increased to above  $k_1 = 0.1$ ,  $M$  and  $C_M$  again decrease because for higher  $k_1$ , it cannot be possible to deliver the needed concentration lower than  $S$  for the successful delivery of molecular bit 0. Therefore,  $M$  and  $C_M$  again decrease. Thus, for  $k_1$  which is very higher than  $S$ , erroneous molecular bits 0 arise and  $M$  and  $C_M$  decrease. Therefore,  $k_1$  should not be a value which is very higher than  $S$  such that erroneous bits can be minimized and  $M$  and  $C_M$  can be maximized.

In Fig. 4,  $M$  is shown with varying  $P_A$  for different  $k_{-1}^0$ . As given in (7), release rate  $k_{-1}$  is directly proportional with  $k_{-1}^0$ . For this analysis,  $k_1 = 0.02$  is used. When  $k_{-1}^0 = 0.001 - 0.01$ ,  $k_{-1}^0$  is smaller than  $k_1$ . Therefore, for molecular bit A, the needed concentration higher than  $S$  can be easily delivered to RN. However, while  $P_A$  increases, the needed concentration smaller than  $S$  cannot be achieved for molecular bit 0 because the concentration of delivered molecules increases while  $P_A$  increases. Thus,  $M$  and  $C_M$  decrease for higher  $P_A$ . When  $k_{-1}^0 = 0.03$ ,  $k_{-1}^0$  is considerably higher than  $k_1$  and the needed concentration smaller than  $S$  can be achieved for molecular bit 0 at higher  $P_A$ .

$$\begin{aligned}
M = & -\left(P_A \frac{E[N_{TA}]}{S} + (1 - P_A) \left(1 - \frac{S}{E[N_{T0}]}\right)\right) \log\left(P_A \frac{E[N_{TA}]}{S} + (1 - P_A) \left(1 - \frac{S}{E[N_{T0}]}\right)\right) - \\
& -\left(P_A \left(1 - \frac{E[N_{TA}]}{S}\right) + (1 - P_A) \frac{S}{E[N_{T0}]} \right) \log\left(P_A \left(1 - \frac{E[N_{TA}]}{S}\right) + (1 - P_A) \frac{S}{E[N_{T0}]} \right) - \\
& -P_A \left(\frac{E[N_{TA}]}{S} \log\left(\frac{E[N_{TA}]}{S}\right) - \left(1 - \frac{E[N_{TA}]}{S}\right) \log\left(1 - \frac{E[N_{TA}]}{S}\right)\right) - \\
& -\left(1 - P_A\right) \left(\frac{S}{E[N_{T0}]} \log\left(\frac{S}{E[N_{T0}]}\right) - \left(1 - \frac{S}{E[N_{T0}]}\right) \log\left(1 - \frac{S}{E[N_{T0}]}\right)\right)
\end{aligned} \tag{18}$$

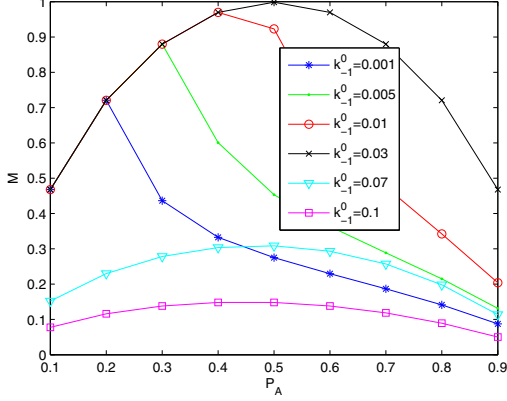


Figure 4:  $M$  with varying  $P_A$  for different  $k_{-1}^0$ .

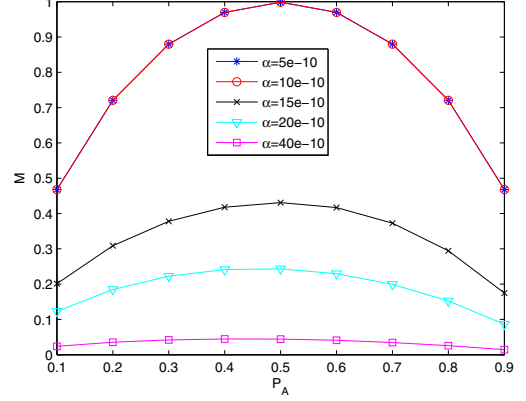


Figure 5:  $M$  with varying  $P_A$  for different  $\alpha$ .

Thus,  $M$  and  $C_M$  is increased and maximized using appropriate  $P_A$ . For  $k_{-1}^0 = 0.07 - 0.1$ ,  $k_{-1}^0$  is much higher than  $k_1$ . In this case, the capability of molecule capturing of RN is very low and the needed concentration higher than  $S$  cannot be delivered for molecular bit  $A$ . Thus,  $M$  and  $C_M$  again decrease. Hence, we can say that  $k_{-1}^0$  should be selected as a value which is considerably higher than  $k_1$  such that  $M$  and  $C_M$  can be maximized.

In Fig. 5,  $M$  is shown with varying  $P_A$  for different  $\alpha$ . For  $\alpha = 5 \times 10^{-10} - 10 \times 10^{-10}$ ,  $M$  and  $C_M$  are higher and can be maximized using appropriate  $P_A$  since smaller distances enable TN to deliver sufficient information to RN by means of appropriate rates  $k_1$  and  $k_{-1}$ . However, while  $\alpha$  increases from  $15 \times 10^{-10}$  to  $40 \times 10^{-10}$ ,  $k_{-1}$  increases and  $k_1$  decreases, then TN cannot achieve to deliver the concentration higher than  $S$  for molecular bit  $A$ . Therefore,  $M$  and  $C_M$  decrease. Hence, it can be said that  $\alpha$  must be selected as an appropriate value to achieve higher molecular communication capacity.

In Fig. 6,  $M$  is shown with varying  $P_A$  for different  $L_{ex}$ . For  $L_{ex} = 0.4 - 2.5$ ,  $L_{ex}$  is sufficiently high such that TN can achieve to deliver the needed concentration to RN for molecular bits  $A$  and  $0$ . Therefore, higher  $M$  and  $C_M$  can be achieved and they can be maximized using appropriate  $P_A$ . However, for  $L_{ex} = 0.05 - 0.2$ , TN cannot achieve to deliver the needed concentration to RN for molecular bits  $A$  and  $0$  and  $M$  and  $C_M$  decrease. Therefore, to achieve higher molecular communication capacity,  $L_{ex}$  must be selected as an appropriate value. Furthermore, if we assume that TN consumes more energy while  $L_{ex}$  increase, in terms of energy consumption after certain  $L_{ex}$  it is not necessary to increase  $L_{ex}$  to achieve higher molecular communication capacity.

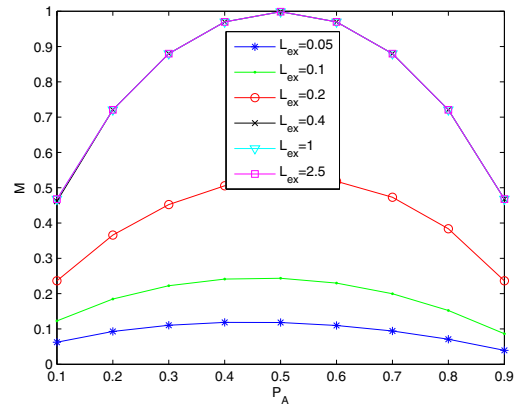


Figure 6:  $M$  with varying  $P_A$  for different  $L_{ex}$ .

Thus, significant energy consumption on TN can be achieved with high molecular communication capacity by selecting appropriate  $L_{ex}$ .

In Fig. 7,  $M$  is shown with varying  $P_A$  for different  $t_H$ . As shown in Fig. 7, for  $t_H = 0.5$ , maximum  $M$  and  $C_M$  can be obtained. However, while  $t_H$  increases,  $M$  and  $C_M$  decreases at higher values of  $P_A$ . The reason for this is that while  $t_H$  and  $P_A$  increases, TN can deliver high concentration to RN such that in transmission of molecular bit  $0$  TN cannot achieve the concentration smaller than  $S$ . Therefore, while  $t_H$  increases, erroneous molecular bit  $0$  arises at higher  $P_A$ . Hence, appropriate  $t_H$  is needed to achieve higher molecular communication capacity.

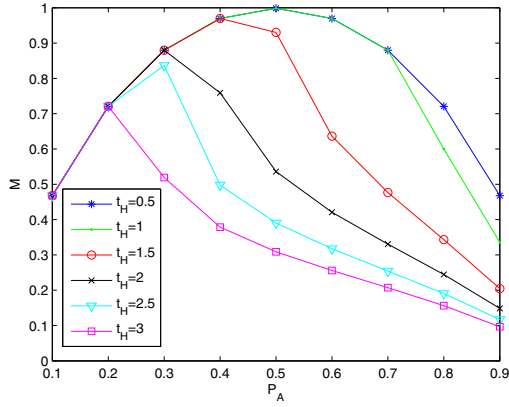


Figure 7:  $M$  with varying  $P_A$  for different  $t_H$ .

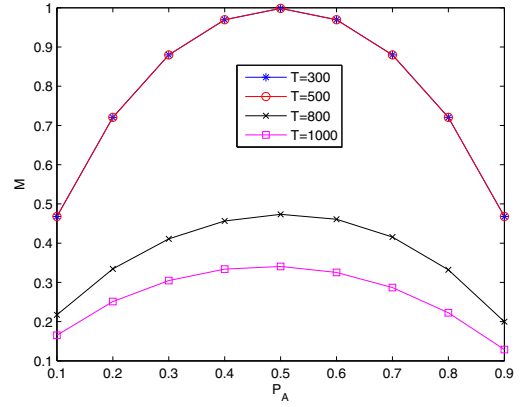


Figure 9:  $M$  with varying  $P_A$  for different  $T$ .

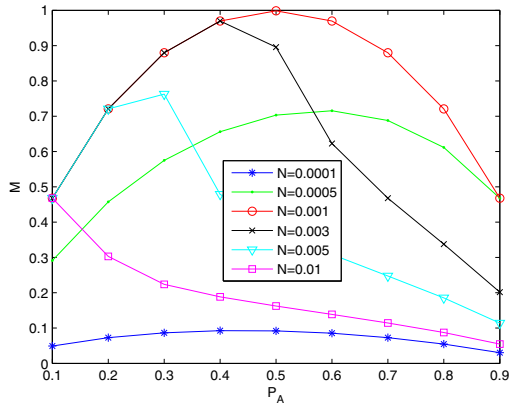


Figure 8:  $M$  with varying  $P_A$  for different  $N$ .

In Fig. 8,  $M$  is shown with varying  $P_A$  for different  $N$ . For  $N = 0.0001 - 0.0005$ , since the concentration of receptors on RN is very small, TN cannot achieve to deliver sufficient molecule concentration for successfully delivery of molecular bit  $A$  such that  $M$  and  $C_M$  are very small for  $N = 0.0001 - 0.0005$ . For  $N = 0.001 - 0.003$ , since the concentration of receptors on RN is sufficient to enable TN to deliver sufficient molecular concentration for molecular bit  $A$  and therefore,  $M$  and  $C_M$  are higher. However, for  $N = 0.005 - 0.01$  the concentration of receptors on RN is very high such that TN delivers very high concentration to RN. In this case, TN delivers the concentration higher than  $S$  for delivery of molecular bit 0 and therefore, erroneous molecular bit 0 arise and  $M$  and  $C_M$  decrease. Thus, it is imperative to select appropriate concentration of  $N$  for higher molecular communication capacity.

In Fig. 9,  $M$  is shown with varying  $P_A$  for different  $T$ . As shown in Fig. 9, for  $T = 300 - 500$ , maximum  $M$  and  $C_M$  can be achieved. While  $T$  increases,  $M$  and  $C_M$  decrease. The reason for this is that while  $T$  increases,  $k_{-1}$  decreases and  $k_1$  increases such that TN can deliver higher molecules. In this case, for transmission of molecular bit 0 TN cannot achieve to deliver the concentration smaller than  $S$ . Therefore, while  $T$  increases,  $M$  and  $C_M$  decrease. Hence, temperature of the environment is also important to achieve higher molecular

communication capacity.

## 6. CONCLUSION

In this paper, we develop an information theoretical approach for capacity of a molecular channel between two nanomachines. We first introduce a molecular communication model. Based on this model, we give molecule delivery approach for the molecular communication between two nanomachines called as Transmitter Nanomachine (TN) and Receiver Nanomachine (RN). Then, we derive a closed form expression for capacity of the channel between TN and RN. According to the capacity expression, we investigate how the conditions such as temperature of environment, concentration of emitted molecules, distance between nanomachines and duration of molecule emission, binding and release rates, concentration of receptors affect the molecular communication capacity. Then, we discuss under which conditions the molecular communication can be feasible and can achieve which capacity. Numerical results shows that selecting appropriate molecular communication parameters such as temperature of environment, concentration of emitted molecules, distance between nanomachines and duration of molecule emission, it can be possible to achieve high capacity for the molecular communication between two nanomachines. Thus, this paper reveals that the molecular communication capacity between two nanomachines is heavily affected from the environmental factors such that appropriate coding and error control mechanisms for molecular communication must consider the environmental factors.

As an extension of this paper, our ongoing works include adaptive coding and error control schemes for the molecular communication channel which can enable high molecular communication capacity with minimum molecular bit error rate according to changing environmental factors such as temperature, diffusion coefficients and distance between the nanomachines. Furthermore, our ongoing researches aim to enable multihop molecular communication between nanomachines which can allow a nano-scale communication network.

## 7. ACKNOWLEDGMENTS

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