On Channel Capacity and Error Compensation in Molecular Communication

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Abstract. Molecular communication is a novel paradigm that uses molecules as an information carrier to enable nanomachines to communicate with each other. 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 communication capacity of the molecular channel. In this paper, we develop an information theoretical approach for capacity of a molecular channel between two nanomachines. Using the principles of mass action kinetics, we first introduce 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. Furthermore, we propose an adaptive Molecular Error Compensation (MEC) scheme for the molecular communication between TN and RN. MEC allows TN to select an appropriate molecular bit transmission probability to maximize molecular communication capacity with respect to environmental factors such as temperature and distance between nanomachines. Numerical analysis show that selecting appropriate molecular communication parameters such as concentration of emitted molecules, duration of molecule emission, and molecular bit transmission probability it can be possible to achieve high molecular communication capacity for the molecular communication channel between two nanomachines. Moreover, the numerical analysis reveals that MEC provides more than % 100 capacity improvement in the molecular communication selecting the most appropriate molecular transmission probability.

Keywords: Molecular communication, nanomachines, molecular bit, information theory, channel capacity, error compensation.

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 functions in

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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].

As in nature, molecular communication is also indispensable to enable nano-scale machines to communicate with each other. Nanotechnology is one of the most important promising technology which enables nano-scale machines called as nanomachines. Nanomachines are molecular scale objects that are capable of performing simple tasks such as actuation and sensing [1]. Nanomachines are categorized into two types. 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.

Due to size and capabilities of nanomachines, the traditional wireless communication with electromagnetic waves cannot be possible to communicate nanomachines that constitute of just several hundreds of atoms or molecules [1]. Instead, the molecular communication is a viable communication paradigm, which enables nanomachines to communicate with each other using molecules as information carrier [1]. Therefore, a molecular channel is envisioned as a communication channel for the molecular communication between two nanomachines. For this channel, it is essential to find out molecular delivery capacity between two nanomachines to understand how to enable molecular communication with high molecule delivery capacity. The molecule delivery capacity may be affected by some parameters specific to the nanomachines and physical properties of the environment such as diffusion coefficient and temperature. Therefore, it is imperative to find out capacity of the molecular channel and to understand how it varies with the properties of the nanomachines and environment.

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 performed. 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 on 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 and propose a closed form expression for molecular communication capacity between two nanomachines and propose an adaptive error compensation technique for molecular communication by significantly extending our preliminary work in [8]. 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. In this paper, we also propose an adaptive Molecular Error Compensation (MEC) scheme for the molecular communication between TN and RN. We first define an interval for selection of the most appropriate molecular bit transmission probability providing higher molecular communication capacity with minimum error. Then, using this interval, we introduce a selection strategy to enable TN to select the most appropriate molecular bit transmission probability with respect to some environmental factors such as temperature, binding rate, and distance between nanomachines. MEC allows TN and RN to collaboratively select the most appropriate molecular bit transmission probability providing high molecular communication capacity. Finally, using the capacity expression and the error compensation scheme, 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 and molecular bit transmission probability that provides higher molecular communication capacity. We further discuss under which conditions the molecular communication can be feasible with high 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 propose an adaptive error compensation scheme. In Section 6, we provide the numerical results and we give concluding results in Section 7.

2 Molecular Communication Model

In nature, molecular communication among biological entities 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 to the receptors of

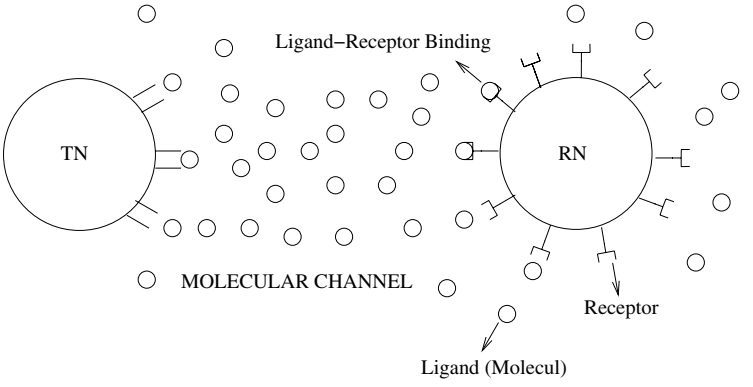


Fig. 1. Molecular Communication Model

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 analogous to the biological mechanisms and 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 [9], [10]. In this paper, we assume an artificial ligand-receptor binding model developed in [9]. 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 a time-varying concentration of $L(t)$ according to the following emission pattern [10] which is similar to alternating square pulse, i.e.,

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

where $j = (0, 1, ...)$, t_H is the duration of a pulse 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 either emits 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 receives a concentration of molecules A greater than a prescribed concentration S ($\mu mol/liter$), the RN decides that the TN transmitted molecular bit A during the time interval t_H. Conversely, if the RN receives molecules A with a concentration less than S, the RN decides that the TN transmitted molecular bit 0.

In traditional digital communication, noise level in the channel leads to 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 observe 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 for RN to receive molecular bit 0 although TN transmits molecular bit A. Moreover, erroneous molecular bits can arise due to some additional 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.

Consequently, 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 approach introduced here.

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, assuming the

ligand-receptor binding model in [9], we introduce a molecule delivery model for the molecular communication between TN and RN.

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

$$A + R \overset{k_1}{\rightarrow} C \tag{2}$$

where k_1 ($\mu mol/liter/sec.$) is the 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,

$$A + R \overset{k_{-1}}{\leftarrow} C \tag{3}$$

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

As given in (1), TN emits molecules A via a square pulse with amplitude L_{ex} during t_H ($sec.$). In this duration, concentration of bound receptors $C(t)$ ($\mu mol/liter$) can be given [9] as follows

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

where k_1 and k_{-1} are the binding and release rates, respectively, L_{ex} ($\mu mol/liter$) is concentration of molecules A which is emitted by TN. C_{∞} is steady-state level of bound receptors and can be given [9] as follows

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

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

During the pulse duration t_H, $C(t)$ rises exponentially according to (4). At time t_0 when the pulse duration ends, $C(t)$ starts to decay [9] according to

$$C(t) = C_{t_0} e^{[-k_{-1}(t-t_0)]} \; for \; t > t_0 \tag{6}$$

The rates of molecule/receptor interaction, k_1 and k_{-1}, may 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 only assume that binding rate (k_1)[1] is inversely proportional with distance (α) 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

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

[1] 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 [14]. However, this is out of scope of this paper.

where k_{-1}^0 is the zero-force release rate, α 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, the distance between TN and RN, and the environmental factors [13]. 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 the properties of RN receptors.

Based on the models introduced in Section 2 and 3, we next develop an information theoretical approach for the capacity of the molecular channel between TN and RN. According to total concentration of complex molecules ($C(t)$) expressed in (4), (5) and (6), we derive probability of erroneous molecular bits which cannot be successfully delivered to RN. Then, we model the molecular communication channel similar to binary symmetric channel and we derive a capacity expression 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 the success of the transmission. If TN transmits molecular bit A, at least S number of molecules[2] 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 the 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), the closed form expressions for expected value of number of delivered molecules A during t_H, i.e., N_A, can be given by

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

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

Since the molecular diffusion continues after every t_H interval, the previous molecular bits can be received in the current interval by RN. Therefore, the number of delivered molecules A in a given interval also depends on molecular bits transmitted in the previous intervals. Here, we assume that the last molecular

[2] Since concentration of molecules ($\mu mol/liter$) can be converted to number of molecules by multiplying Avagadro constant (6.02×10^{23}), we interchangeably use the number of molecules for the concentration of molecules.

bit only affects the current molecular transmission since the number of delivered molecules exponentially decay after t_H seconds according to (6). If we assume that TN emits molecules A with probability P_A in each time interval t_H and it emits molecular bit 0 with probability $(1-P_A)$. Hence, the effect of the last emitted molecular bit on the current molecular bit transmission can be considered as expected number of delivered molecules coming from the previous interval, i.e., N_p. Thus, using (6) and (9), N_p can be given as follows

$$N_p = \int_0^{t_H} P_A N_A e^{(-k_{-1}t)} dt \tag{10}$$

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

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

$$E[N_{TA}] = N_A + N_p \tag{12}$$

At the RN side, if RN receives 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 obtain a maximum bound for the probability p_1 that TN achieves to deliver molecular bit A as follows

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

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), the expected value of total number of delivered molecules A within t_H for the transmission of molecular bit 0, i.e., $E[N_{T0}]$, is given by

$$E[N_{T0}] = N_p \tag{14}$$

For the successful delivery of a molecular bit 0, TN must deliver a number of molecules A that is less than S and $(N_{T0} \leq S)$ to RN. Using the Markov inequality, the maximum bound for probability p_2 that TN achieves to deliver molecular bit 0 is given by

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

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 $(1 - p_2)$. Here, it is critical to select an appropriate S to maximize p_1 and p_2. As seen in (13), for $E[N_{TA}] \geq S$, $p_1 \geq 1$ is obtained although it is not possible for p_1 to take a value greater than 1. This implies that $p_1 \approx 1$ can be obtained by appropriately selecting S. For example, if we assume that N_{TA} is a random variable with the normal distribution $N(E[N_{TA}], \sigma_{TA}2)$, $p_1 \approx 1$ can be obtained by selecting S as $0 < S < E[N_{TA}] - 3\sigma_{TA}$. This is because in any normal distribution, % 99.7 of the observations fall within 3 standard deviations of the mean. Similarly, if we assume that N_{T0} has the normal distribution $N(E[N_{T0}], \sigma_{T0}2)$, $p_2 \approx 1$ can be succeed selecting S as $S > E[N_{T0}] + 3\sigma_{T0}$. Consequently, p_1 and p_2 can be maximized by selecting S from the interval $0 < E[N_{T0}] + 3\sigma_{T0} < S < E[N_{TA}] - 3\sigma_{TA}$

According to the transmission probabilities p_1 and p_2, we can model a channel similar to the symmetric channel [15]. 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

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

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

$$M = \Big(H\Big(p_1 P_A + (1-p_2)(1-P_A), (1-p_1)P_A + p_2(1-P_A)\Big)\Big) - \\ - \Big(P_A H(p_1, 1-p_1) + (1-P_A)H(p_2, 1-p_2)\Big) \tag{16}$$

$$\begin{aligned} M = & -\Big[P_A \tfrac{E[N_{TA}]}{S} + \big(1-P_A\big)\big(1-\tfrac{S}{E[N_{T0}]}\big)\Big] log\Big[P_A \tfrac{E[N_{TA}]}{S} + \big(1-P_A\big)\big(1-\tfrac{S}{E[N_{T0}]}\big)\Big] - \\ & -\Big[P_A\big(1-\tfrac{E[N_{TA}]}{S}\big) + \big(1-P_A\big)\tfrac{S}{E[N_{T0}]}\Big] log\Big[P_A\big(1-\tfrac{E[N_{TA}]}{S}\big) + \big(1-P_A\big)\tfrac{S}{E[N_{T0}]}\Big] - \\ & -P_A\Big[\tfrac{E[N_{TA}]}{S} log\big(\tfrac{E[N_{TA}]}{S}\big) - \big(1-\tfrac{E[N_{TA}]}{S}\big) log\big(1-\tfrac{E[N_{TA}]}{S}\big)\Big] - \\ & -\big(1-P_A\big)\Big[\tfrac{S}{E[N_{T0}]} log\big(\tfrac{S}{E[N_{T0}]}\big) - \big(1-\tfrac{S}{E[N_{T0}]}\big) log\big(1-\tfrac{S}{E[N_{T0}]}\big)\Big] \end{aligned} \tag{17}$$

where $H(.)$ denotes the entropy. Using (17), the capacity of the molecular channel between TN and RN i.e., C_M, can be expressed as

$$C_M = max(M) \tag{18}$$

Traditionally, in a communication channel it is necessary to design codes that enable minimum error rate and maximum capacity. Similarly, in a molecular communication channel, it is necessary to find a molecular bit transmission probability that can maximize molecular communication capacity. Next, we introduce

an adaptive error compensation scheme in the molecular communication, which enable TN to select most appropriate molecular bit transmission probability that can maximize molecular communication capacity.

5 Adaptive Error Compensation in the Molecular Communication

In the traditional digital communication, erroneous bits are frequently observed due to noise in the channel. To compensate bit errors, various kinds of channel coding schemes have been proposed in the literature. Generally, the aim of these techniques is to reduce bit error probability of communication between transmitter and receiver. For this aim, transmitter organizes transmitting communication bits to generate fixed-length codewords such that these codewords enable the receiver to detect and correct the erroneous communication bits. However, detection and correction of erroneous communication bits necessitate efficient processors, algorithms, and circuits with high computational power at the receiver side.

As in traditional digital communication, two molecular communication bits are available for the communication between TN and RN. However, existing channel coding techniques are not appropriate for the molecular communication since they necessitate high computational power, which may not be realizable for nanomachines with limited computational and storage capabilities. Therefore, the molecular communication needs proactive error compensation schemes, which do not necessitate any computational processing to compensate possible errors on the molecular channel. These error compensation schemes should proactively prevent the possible errors on the molecular communication channel by adapting some molecular communication parameters according to changing environmental factors such as temperature, binding rate, and distance between nanomachines.

In the molecular communication, we assume that some communication parameters such as concentration of emitted molecules A (L_{ex}), duration of emission pulse (t_H), and concentration of receptors on RN (N) are specific to the TN and RN and related with the design issues of the nanomachines. Therefore, they cannot be changed by neither nanomachines nor environmental factors. However, other parameters such as temperature of the environment (T), applied force per bound (f), distance between TN and RN (α), binding rate (k_1), release rate (k_{-1}), and zero-force release rate (k^0_{-1}) only depend on some environmental factors such as diffusion coefficients of the environment and deployment strategies of the nanomachines. Here, we assume that the probability of molecular bit A emission (P_A) can only be changed by TN. Therefore, a proactive error compensation scheme exploits regulation of P_A such that the regulation can proactively compensate the possible channel errors, which stem from some environmental factors and some properties of the nanomachines. For example, in an environment generating high binding rate (k_1), transmission of molecular bit 0 can be erroneous since high amount of molecules A can be delivered to RN during the

transmission of molecular bit 0. However, selection of the most appropriate P_A decreasing the number of delivered molecules can enable TN to compensate such kind of errors.

Theoretically, it is possible to optimize (17) to find a molecular transmission probability (P_A), which minimizes the errors on molecular communication channel and maximizes molecular communication capacity. This can enable TN to encode transmitted molecular bit such that TN can minimize the errors. However, this kind of optimization process is computationally impossible for TN. In stead of some optimization process with high computational burden, it is possible to find some simple methods that enable TN to decide which P_A is the most appropriate in which environmental conditions.

According to the molecular communication model introduced in Section 2, to successfully deliver molecular bit A TN must deliver at least S number of molecules A to RN. Therefore, the condition

$$E[N_{TA}] = N_A + N_p > S \tag{19}$$

must hold for successful delivery of molecular bit A. Substituting N_p given in (10), we rewrite (19) as

$$N_A + P_A N_A \int_0^{t_H} e^{(-k_{-1}t)} dt > S \tag{20}$$

Using (20), a lower bound for P_A, i.e., LB, can be given as

$$P_A > \frac{S - N_A}{N_A \int_0^{t_H} e^{(-k_{-1}t)} dt} = LB \tag{21}$$

where $N_A \int_0^{t_H} e^{(-k_{-1}t)} dt$ states concentration of molecules A that are received by RN within an exponential decaying phase after TN transmits molecular bit A as introduced in (11). We denote $N_A \int_0^{t_H} e^{(-k_{-1}t)} dt$ with N_{ex} and rewrite (21) as

$$LB = \frac{S - N_A}{N_{ex}} \tag{22}$$

To successfully deliver molecular bit 0, TN must deliver a number of molecules A less than S to RN. Therefore, the condition that must be met for successful delivery of molecular bit 0 is expressed as

$$E[N_{T0}] = N_p \leq S \tag{23}$$

where $E[N_{T0}]$ and N_p denote the expected number of delivered molecules coming from the previous interval as introduced in (10). Using (10), (23) can be rewritten as

$$P_A N_A \int_0^{t_H} e^{(-k_{-1}t)} dt \leq S \tag{24}$$

Similar to lower bound given in (22), using (24), an upper bound for P_A, i.e., UB, can be given as follows

$$P_A \leq \frac{S}{N_A \int_0^{t_H} e^{(-k_{-1}t)} dt} = UB \tag{25}$$

$$UB = \frac{S}{N_{ex}} \tag{26}$$

Combining the lower and upper bounds given in (22) and (26), respectively, an interval for selection of the most appropriate P_A that minimizes the channel errors in the molecular communication can be stated as

$$\frac{S - N_A}{N_{ex}} < P_A \leq \frac{S}{N_{ex}} \tag{27}$$

$$LB < P_A \leq UB \tag{28}$$

N_{ex} includes an integral operation that is impossible for TN to practically compute due to its very limited computational power. Since N_{ex} states concentration of molecules A that are received by RN within an exponential decaying phase after TN transmits molecular bit A, RN can obtain N_{ex} by computing concentration of molecules A within an exponential decaying phase after TN transmits a molecular bit A. Here, we assume that similar to the molecular communication from TN to RN, molecular communication from RN to TN can be possible[3]. We also assume that RN computes the concentration within an exponential decaying phase after TN transmits a molecular bit A and it communicates this concentration to RN before initiating the molecular communication. Thus, to determine an appropriate P_A providing satisfactory molecular communication capacity, TN evaluates the lower and upper bounds given in (27). However, TN needs a selection strategy to select the most appropriate molecular bit transmission probability (P_A) from the interval given in (28).

5.1 A Selection Strategy for Molecular Bit Transmission Probability

For the molecular communication, it is critical to select the most appropriate molecular bit transmission probability (P_A) providing high molecular communication capacity. Using the interval given in (27), we investigate how the variation of P_A affects the error rate in the molecular communication such that we derive a selection strategy for P_A, which allows TN to minimize error rate and to maximize molecular communication capacity.

While P_A increases, the number of delivered molecules increases. Therefore, higher P_A decreases the errors in transmission of molecular bit A. Conversely, while P_A increases, errors increase in transmission of molecular bit 0. However, P_A less than UB enables non-erroneous molecular bit 0 transmission as introduced in derivation of UB. Therefore, P_A should be selected as high as possible for non-erroneous molecular bit A transmission while it should be selected less than UB for non-erroneous molecular bit 0. Hence, P_A should be selected as a value that is the closest to UB ($P_A \cong UB$). This selection strategy can minimize

[3] Here, we also note that TN and RN have the same molecule delivery and reception capability. However, we do not assume full duplex molecular communication between TN and RN such that TN and RN cannot simultaneously deliver or receive molecular bits. Hence, we assume a half duplex molecular communication between TN and RN.

error rate and maximize molecular communication capacity. According to this P_A selection strategy, UB is more important than LB because $P_A \cong UB$ can provide higher molecular communication capacity. Therefore, in the numerical analysis in Section 6 we evaluate only UB for the selection of P_A.

5.2 An Adaptive Molecular Error Compensation Scheme

In the molecular communication, error rate is heavily affected by some environmental factors such as binding rate (k_1), temperature (T), distance (α) between nanomachines. Therefore, it is imperative to compensate the errors due to the changing environmental factors to achieve higher molecular communication capacity. For this compensation, it is essential to regulate molecular bit transmission probability (P_A) with respect to the changing environmental factors. However, the regulation of P_A to compensate the errors needs some coordination between TN and RN. This coordination enables an adaptive error compensation scheme that is periodically conducted by TN and RN to compensate possible channel errors. Here, we introduce an adaptive Molecular Error Compensation (MEC) scheme for the molecular communication between TN and RN as outlined below:

1. Initially, TN sets the molecular bit transmission probability P_A to an initial value denoted by $\overline{P_A}$ and initiates the molecular communication.
2. When error rate increases, RN detects the increasing error rate[4].
3. RN emits a molecular bit stream denoted by BS_1 to terminate current molecular communication between TN and RN and to initiate the error compensation scheme. BS_1 is a special stream[5] such that when it is received by TN, TN can immediately terminate the current molecular communication and infer the initiation of the error compensation scheme. Therefore, by means of BS_1, RN can initiate the error compensation scheme in any time when it detects increasing error rate in the molecular channel.
4. Once TN receives BS_1, it immediately emits the molecular bit stream BS_2 [6] like $A00000A00000$ to enable RN to compute N_{ex} and UB.
5. Using N_{ex} and UB, RN selects P_A as a value closest to UB ($P_A \cong UB$).
6. RN informs TN about the selected molecular bit transmission probability. Here, we do not assume that RN communicates the actual value of the selected P_A, which is possibly a floating point number, to TN. We only assume that RN emits specific molecular bit patterns corresponding to the different level of molecular bit transmission probability such that according

[4] Note that while it may be possible to develop some error detection mechanisms for molecular communication, it is beyond the scope of this paper.

[5] BS_1 is a fixed molecular bit stream, which may be determined in the design stage of the molecular communication system. For example, $A0A$ may be selected as BS_1.

[6] Since N_{ex} is the number of molecules delivered within an exponential decaying phase after TN emits A, BS_2 is appropriate to enable RN to compute N_{ex}. Furthermore, other molecular bit streams that can enable this computation can be selected for this computation.

Algorithm 1. MEC

```
1  TN sets P_A as the complement of P_A
2  TN initiates the molecular communication
3  foreach P_A do
4      RN detects the increasing error rate
5      RN emits BS_1
6      TN terminates the molecular communication
7      TN emits BS_2
8      RN computes N_ex and UB
9      RN selects P_A, (P_A ≅ UB)
10     RN informs TN about the selected P_A
11     TN updates P_A as the selected P_A
12     TN emits BS_3
13     TN again initiates the molecular communication
14 end
```

to the emitted molecular bit pattern, TN infers the selected molecular bit transmission probability.

7. TN sets P_A as the selected molecular bit transmission probability. After the setting of the molecular bit transmission probability, TN emits the molecular bit stream BS_3[7] to again initiate the molecular communication. Then, TN again initiates the molecular communication according to the updated molecular bit transmission probability, which minimizes the error rate and maximizes the molecular communication capacity.

Using the adaptive Molecular Error Compensation (MEC) scheme given above, TN and RN can collaboratively select P_A to minimize the error rate and maximize molecular communication capacity. We also give MEC in the pseudo-code given in Algorithm 1.

6 Numerical Analysis

In this section, we first present the numerical analysis performed over the mutual information expression given in (17) to show how the molecular communication capacity varies according to the some environmental parameters and some other parameters specific to the nanomachines TN and RN. Then, we give the numerical analysis for the performance of MEC over the selection of the most appropriate P_A that provides high molecular communication capacity with minimum error rate. The aim of this analysis is to determine appropriate configuration of molecular communication parameters, which can achieve high molecular communication capacity, according to changing environmental factors. We perform the numerical analysis using Matlab. We assume that TN and RN are randomly positioned in an environment, which may have different diffusion coefficients

[7] Similar to BS_1, BS_3 is also a fixed molecular bit stream, which determined in the design. For example, $0A0$ may be selected as BS_3.

Table 1. Simulation Parameters

Binding rate (k_1)	0.1-0.5 $(\mu mol/liter/s)$
Zero-force release rate (k_{-1}^0)	0.08 (s^{-1})
Temperature (T)	300-1000 K
Distance between TN and RN (α)	$5^{-10} - 4 \times 10^{-9} m$
Applied force per bound (f)	10^{-12} (J/m)
Concentration of molecules A (L_{ex})	1-8 $(\mu mol/liter)$
Duration of the pulses (t_H)	0.5-1 s
Number of receptors R (N)	0.001-0.01 $(\mu mol/liter)$
$\boldsymbol{S}$ $(\mu mol/liter)$	$10^{-6} - 4 \times 10^{-6}$

such that it allows TN to achieve different binding rates (k_1). Due to the principles of mass action kinetics, we also assume that k_1 varies with temperature of environment (T) and distance (α) between TN and RN such that k_1 is directly proportional with $2T$ $(k_1 \propto 2T)$ and inversely proportional with α $(k_1 \propto 1/\alpha)$, respectively. Moreover, we assume that k_{-1}^0 depends only on the properties of RN receptors and cannot be changed. The simulation parameters of the analysis are given in Table 1.

6.1 Effect of Environmental Factors on Molecular Communication Capacity

Binding Rate: For the first analysis, we investigate the effect of binding rate (k_1) on capacity of the molecular channel. In Fig. 2, mutual information (M) given in (17) is shown with varying molecular bit transmission probability (P_A) for different k_1. For higher $k_1 = 0.2 - 0.4\ \mu mol/liter/s$, TN delivers higher number of molecules A that is greater than S. Therefore, for higher k_1, transmission of molecular bit 0 can be erroneous and molecular communication capacity decreases. However, for a smaller $k_1 = 0.1\ \mu mol/liter/s$ that enables TN to deliver sufficient molecules for molecular bit A and 0, M can be maximized selecting an appropriate P_A. TN can deliver greater than S number of molecules in transmission of molecular bit A and deliver less than S number of molecules in transmission of molecular bit 0. Therefore, to achieve high molecular communication capacity, it is necessary to select appropriate S with respect to binding rate (k_1). For an environment imposing higher k_1, S should be selected as a sufficiently high value that can hinder the delivery of erroneous molecular bit 0. For an environment imposing smaller k_1, a smaller S should be used such that it can hinder the delivery of erroneous molecular bit A.

Temperature: Temperature of the environment (T) is another important parameter since it heavily affects the binding rate (k_1) and molecular communication capacity. However, T has similar effects with k_1 on the molecular communication capacity. In Fig. 3, M is shown with varying P_A for different T. For $T = 300 - 500\ K$, higher molecular communication capacity can be achieved. However, the capacity decreases while T is further increased from 500 K to 1000 K $(T = 500 - 1000\ K)$. This stems from binding rate (k_1) that increases

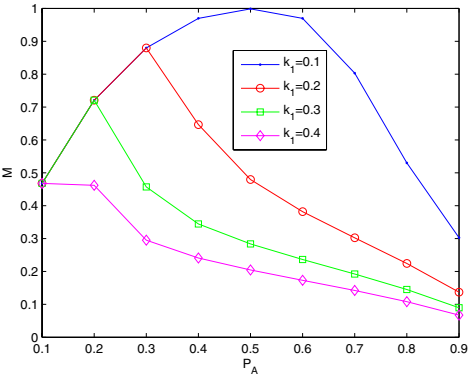


Fig. 2. M with varying P_A for different k_1

with the higher temperature (T) such that the increasing k_1 results in delivery of excessively high number of molecules and erroneous molecular bit 0 and the capacity decreases. Hence, for an environment having higher T, S should be selected as a sufficiently high value to prevent erroneous molecular bit 0 and to maximize molecular communication capacity.

Distance between TN and RN: As the traditional wireless communication, distance (α) between TN and RN heavily affects molecular communication capacity since k_1 depends on α. While α decreases, k_1 increases. To evaluate the effect of α on molecular communication, in Fig. 4, M is shown with varying P_A for different α. For smaller $\alpha = 5 \times 10^{-10} - 20 \times 10^{-10}$ m, k_1 increases and excessive number of molecules that is greater than S is delivered to RN. This results in erroneous molecular bit 0 and decreases the capacity. However, for a sufficiently high $\alpha = 40 \times 10^{-10}$ m providing appropriate k_1, TN delivers a number of molecules less than S in transmission of molecular bit 0 and delivers greater than S number of molecules in transmission of molecular bit A. This can maximize the molecular communication capacity. Therefore, S should be selected with respect to distance between TN and RN. While the distance increases, S should be decreased to prevent erroneous molecular bit A. While the distance decreases, S should be increased to prevent erroneous molecular bit 0.

6.2 Effect of the Parameters Specific to TN and RN on Molecular Communication

In this section, we present the numerical results for effect of some parameters specific to TN and RN. S is one of the most important molecular communication parameter specific to TN and RN. In Fig. 5(a), M is shown with varying P_A for different S. For smaller $S = 1 \times 10^{-6} - 2 \times 10^{-6}$ $\mu mol/liter$, it is most likely that TN can deliver a number of molecules A that is greater than S. Therefore, molecular communication capacity decreases while S decreases. However, using a sufficiently high $S = 3 \times 10^{-6} - 4 \times 10^{-6}$ $\mu mol/liter$, which enables non-erroneous

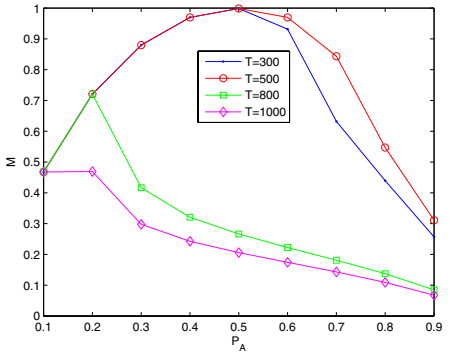


Fig. 3. M with varying P_A for different T

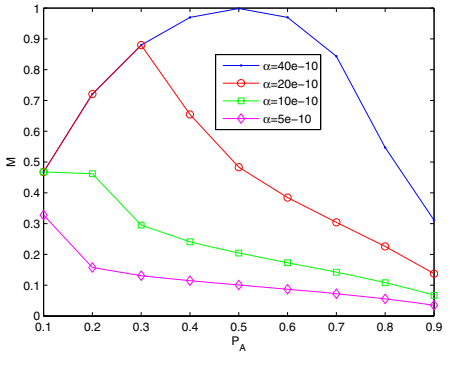
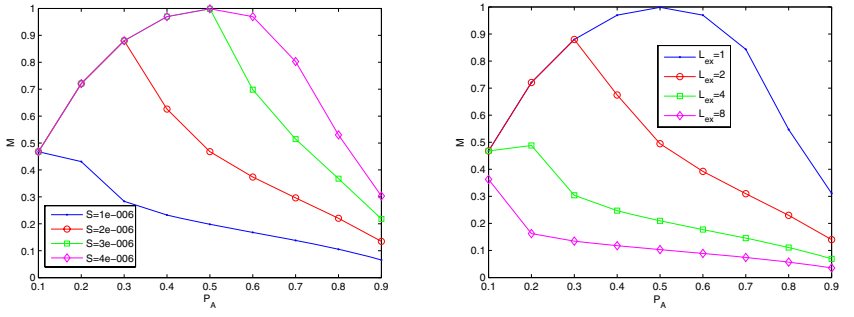


Fig. 4. M with varying P_A for different α

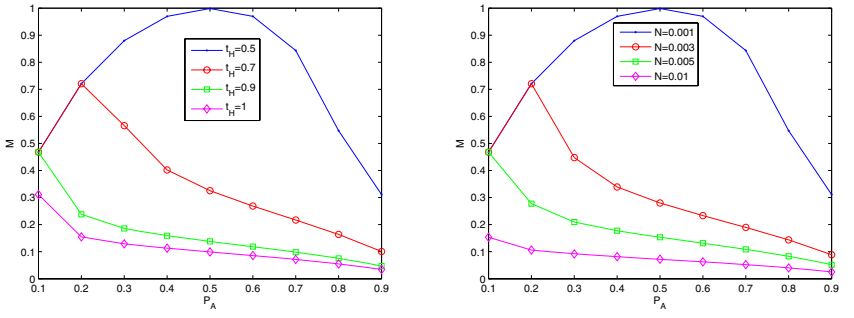
molecular communication bits, maximum molecular communication capacity can be achieved. Hence, S should be selected according to some environmental factors such as binding rate (k_1), temperature (T), and distance between TN and RN (α). For an environment imposing high k_1 and T, S should be used as a smaller value to prevent erroneous molecular bit 0.

Concentration of emitted molecules (L_{ex}) is also one of the most important parameters specific to TN and RN, which affects the number of delivered molecules in each transmission of molecular bits. In Fig. 5(b), M is shown with varying P_A for different L_{ex}. For $L_{ex} = 1\ \mu mol/liter$, L_{ex} is sufficiently high such that TN can achieve to deliver the needed concentration to RN for molecular bits A and 0. Therefore, high molecular communication capacity can be achieved and they can be maximized using appropriate P_A. However, for $L_{ex} = 2 - 8\ \mu mol/liter$, TN delivers excessive concentration to RN for molecular bits 0, which is greater than S and erroneous bits arise and the molecular communication capacity decreases. Therefore, to achieve higher molecular communication capacity, L_{ex} must be selected as an appropriate value according to the environmental factors such as binding rate, temperature and distance between TN and RN.



(a) (b)

Fig. 5. (a) M for different S. (b) M for different L_{ex}.



(a) (b)

Fig. 6. (a) M for different t_H. (b) M for different N.

Duration of emission pulse (t_H) is critical for performance of the molecular communication. While t_H increases, number of delivered molecules increases. Therefore, erroneous molecular bits 0 arise while t_H increases. In Fig. 6(a), M is shown with varying P_A for different t_H. For $t_H = 0.5\ s$, high molecular communication capacity can be achieved. However, the capacity decreases at higher values of P_A while t_H increases. As t_H and P_A increase, number of delivered molecules increases such that TN cannot deliver the concentration smaller than S in transmission of molecular bit 0. Therefore, erroneous molecular bit 0 arises at higher P_A while t_H increases. Hence, appropriate t_H is needed to achieve higher molecular communication capacity.

Concentration of receptors (N) on RN also affects the number of delivered molecules in the molecular communication. While N increases, number of delivered molecules increases. In Fig. 6(b), M is shown with varying P_A for different N. For $N = 0.003 - 0.01\ \mu mol/liter$, TN delivers excessive number of molecules in transmission of molecular bit 0 and erroneous molecular bits arise and the molecular communication capacity decreases. For $N = 0.001\ \mu mol/liter$, the concentration of receptors on RN is sufficient to enable TN to deliver sufficient

molecular concentration for molecular bit A and 0. Therefore, selecting appropriate N, the molecular communication capacity can be maximized. When the environment allows delivery of smaller number of molecules, N should be selected as a higher value to enable TN to deliver sufficient number of molecules for non-erroneous molecular bit A.

6.3 Adaptive Molecular Error Compensation Scheme

In this section, we present the numerical analysis on performance of adaptive Molecular Error Compensation (MEC) scheme. For the performance of MEC, we show the mutual information given in (17) with and without MEC scheme according to the varying environmental factors with higher error rate. For the case with MEC, we allow MEC scheme to select molecular transmission probability (P_A) to compensate possible molecular errors and to achieve high molecular communication capacity according to varying environmental factors. For the case without MEC, we statically set P_A as $P_A = 0.5$ regardless of changing environmental factors. We show the effect of MEC on the molecular communication capacity in terms of variation of three environmental factors, binding rate (k_1), temperature (T), and distance between TN and RN (α). Throughout the analysis, MEC sets molecular transmission probability (P_A) as $P_A = \lfloor 10UB \rfloor /10$, where $\lfloor . \rfloor$ denotes the floor function. This selection strategy provides an appropriate P_A for MEC such that $P_A \cong UB$.

Binding Rate: In Fig. 7, mutual information (M) given in (17) is shown for varying binding rate (k_1) with and without MEC. As k_1 increases ($k_1 = 0.1 - 0.5\ \mu mol/liter/s$), molecular communication capacity decreases due to erroneous molecular bit 0. However, MEC can compensate some possible errors selecting the most appropriate P_A. MEC provides % 100 capacity improvement with repect to the case that statically selects $P_A = 0.5$ without MEC.

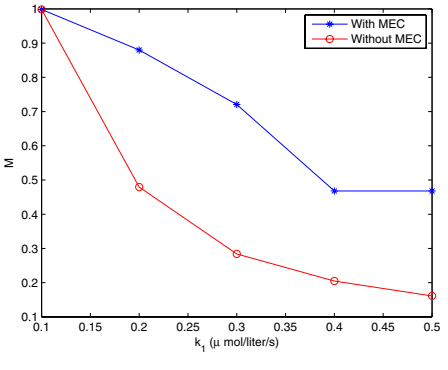


Fig. 7. M for varying k_1 with and without MEC

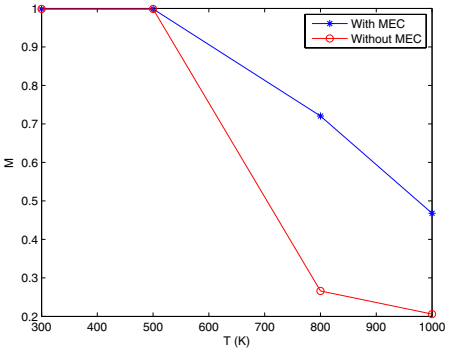


Fig. 8. M for varying T with and without MEC

Temperature: In Fig. 8, M is shown for varying temperature (T) with and without MEC. While T increases, the molecular communication capacity decreases due to increasing error rate in transmission of molecular bit 0. For $T = 300 - 500\ K$, almost the same capacity can be achieved with and without MEC because $\lfloor 10UB \rfloor / 10 \cong 0.5$. However, as T further increases, MEC significantly overcomes the static selection strategy in which P_A is set as $P_A = 0.5$ selecting the most appropriate P_A and MEC can compensate possible errors and achieve high molecular communication capacity.

Distance between TN and RN: In Fig. 9, M is shown for varying distance between TN and RN (α). As α decreases, the molecular communication capacity decreases due to increasing error rate in transmission of molecular bit A. However, MEC can compensate these errors and achieve high molecular communication capacity selecting the most appropriate P_A. MEC provides more than % 100 capacity imporvement with respect to the static selection strategy using $P_A = 0.5$.

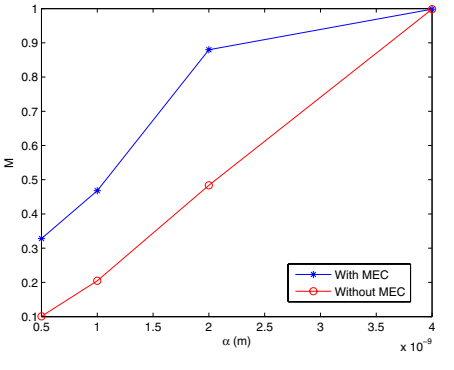


Fig. 9. M for varying α with and without MEC

7 Conclusion

In this paper, we derive a closed form expression for capacity of the channel between TN and RN. Furthermore, we propose an adaptive Molecular Error Compensation (MEC) scheme for the molecular communication between TN and RN. MEC allows TN and RN to collaboratively select the most appropriate appropriate molecular bit transmission probability to maximize molecular communication capacity with respect to environmental factors such as temperature, binding rate, distance between nanomachines. Using 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 rate, concentration of receptors affect the molecular communication capacity. Numerical analysis reveals that MEC provides more than % 100 capacity improvement in the molecular communication selecting the most appropriate molecular transmission probability that proactively compensate the possible errors in the molecular channel. Numerical analysis also shows that the molecular communication with high capacity is only possible by arranging the molecular communication parameters such that cross-relation between the parameters should be carefully considered to compensate their negative effects over each other. Furthermore, a possible design scheme for the molecular communication should consider the environmental factors to provide high molecular communication capacity. The design scheme should select the parameters specific to TN and RN according to the environmental factors.

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