Single and Multiple-Access Channel Capacity in Molecular Nanonetworks

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Abstract. Molecular communication is a new nano-scale communication paradigm that enables nanomachines to communicate with each other by emitting molecules to their surrounding environment. Nanonetworks are also envisioned to be composed of a number of nanomachines with molecular communication capability that are deployed in an environment to share specific molecular information such as odor, flavour, light, or any chemical state. In this paper, using the principles of natural ligand-receptor binding mechanisms in biology, we first derive a capacity expression for single molecular channel in which a single Transmitter Nanomachine (TN) communicates with a single Receiver Nanomachine (RN). Then, we investigate the capacity of the molecular multiple-access channel in which multiple TNs communicate with a single RN. Numerical results reveal that high molecular communication capacities can be attainable for the single and multiple-access molecular channels.

Key words: Molecular communication, Nanonetworks, Single molecular channel, Molecular multiple-access channel.

1 Introduction

Molecular communication is a new communication paradigm that enables nanomachines to communicate with each other using molecules as a communication carrier [1]. A number of nanomachines with molecular communication is envisioned as a nanonetwork to cooperatively share molecular information and to achieve a specific task from nuclear, biological, and chemical attack detection to food and water quality control [2]. In a nanonetwork, we define the single and multiple-access molecular channels as follows [7]:

- *Single molecular channel* is a molecular communication channel between a single Transmitter Nanomachine (TN) and a single Receiver Nanomachine (RN).
- *Molecular multiple-access channel* is a molecular communication channel in which multiple TNs transmit molecular information to a single RN.

In the literature, there exist several conceptual studies on the molecular communication paradigm [1, 2, 3]. However, these studies do not investigate the molecular communication from the communication theory perspective. In [4, 5], achievable information rate is investigated in the molecular communication channel that is modeled as a timing channel. The channel model considers Brownian motion as a main mechanism to deliver emitted molecules to the receiver side within a time delay. However, it does not include any realistic physical parameter such as environment temperature, molecular mass, and diffusion coefficients that are main determinant for the molecular delivery time and its fluctuations. Moreover, the molecular communication channel modeled as the timing channel may necessitate the nanomachines to strictly synchronize with each other and also incur high computational burden for the nanomachines, which may also be impractical for low-end nanomachines.

In our previous work [6], we model the single and multiple-access molecular channels as a binary symmetric channel with two molecular communication bits corresponding to a specific molecule concentration delivered to RN by TNs. This approach severely restricts the molecular communication capacity to one bit per transmission. However, the single and multiple-access molecular channels may deliver more than one concentration level corresponding to higher molecular communication rates instead of a specific concentration level and two corresponding molecular communication bits. Therefore, the capacity of the single and multiple-access molecular channels need to be further investigated to find out their actual capacity expressions. In this paper, using the principles of natural ligand-receptor binding mechanisms in biology, we first derive the capacity of the single molecular channel in Section 2. Then, we find out the capacity of the molecular multiple-access channel in Section 3. In Section 4, we give the numerical results on the capacity of the single molecular channel and molecular multiple-access channel. Finally, we give concluding remarks in Section 5.

2 Single Molecular Communication Channel

In nature, biological entities communicate with each other via the ligand-receptor binding mechanism, in which ligand molecules are emitted by one biological phenomenon then, the emitted ligand molecules bind to the receptors of another biological phenomenon. According to the bound molecule concentration, the biological phenomenon perceives the biological information and to fire an action potential. Hence, biological molecular channel can be envisaged as a *concentration channel*. In this paper, we use the natural ligand-receptor binding mechanism to model the molecular communication between TN and RN[1] and we consider this molecular communication channel as a concentration channel. In the literature, artificial ligand-receptor binding schemes have been previously

[1] Here, we assume that TN and RN are analogous to the biological mechanisms such as a single cell or a bacteria and have spherical shape with radius r_0.

introduced in [8], [9], [10]. In this paper, we assume an artificial ligand-receptor binding model introduced in [10].

We assume that TN emits one kind of molecule called A with concentration X ($\mu mol/liter$) and X is a random variable with the mean μ_x and the variance σ_x^2. Furthermore, we assume that RN has the receptors called R on its surface with constant concentration N ($\mu mol/liter$). The receptors enable RN to receive the molecules which bind to their surface. When TN emits molecules A with concentration X, some of molecules bind to these receptors and generate bound molecules with a concentration. Using the ligand-receptor binding model given in [10], the concentration of these bound molecules, i.e., B, can be given as

$$B = \frac{k_1 N X}{k_{-1}} \tag{1}$$

where k_1 and k_{-1} are the constant binding and release rate, respectively. The binding rate k_1 indicates the ratio of the molecules binding to the receptors on RN while the release rate k_{-1} indicates the ratio of the molecules releasing from the receptors. Here, we assume that k_{-1} is a constant which is affected by physical properties of the receptors on RN and it does not change as long as the physical properties of the receptors on RN do not change. However, k_1 is affected by the several environmental factors such as molecular diffusion coefficients, temperature, and distance between TN and RN. In the literature, there are several realistic models for k_1 that are experimentally tested for certain biochemical reactions [11], [12], [13]. In this paper, we use the following model [11] for k_1,

$$k_1 = \frac{4\pi D r_0 \beta}{1 - (1-\beta)\frac{r_0}{r_\infty}} \tag{2}$$

where D is the diffusion coefficient of the emitted molecules, r_0 (A°) is the radius of RN and r_∞ (A°) is the radius of the spherical shaped environment in which TN and RN communicate. β is the fraction of the molecule trajectories that allow the molecules emitted by TN to bind the receptors on RN. If we assume that the distance between TN and RN is α, the probability that a molecule emitted by TN will be captured by RN can be given as $\frac{r_0}{\alpha}$ [12]. Therefore, we set the fraction of the molecule trajectories that allow the molecules to bind the receptors on RN, i.e., β, as $\beta = \frac{r_0}{\alpha}$.

Since the emitted molecules A continuously diffuse in the environment and the diffusion process can have some natural variations as many natural events, we assume the concentration of bound molecules (B) is exposed to a noise level denoted by Z. Thus, the concentration of molecules delivered to RN by TN, i.e., Y, can be given as

$$Y = B + Z = \frac{k_1 N X}{k_{-1}} + Z \tag{3}$$

where we assume that Z is a random variable with the normal distribution $N(\mu_z, \sigma_z^2)$. Many events in nature can be approximated with the normal distri-

bution corresponding to the central limit theorem. Therefore, this assumption is reasonable to effectively investigate the molecular channel capacity.

Hence, assuming that X and Z are independent random variables, the mutual information of the single molecular channel between TN and RN, i.e., $I(X;Y)$, can be expressed as

$$I(X;Y) = H(Y) - H\left(\left[\frac{k_1 N X}{k_{-1}} + Z\right]|X\right) = H(Y) - H(Z) \tag{4}$$

In order to maximize the mutual information $I(X;Y)$ for providing the capacity of the single molecular channel, $H(Y)$ should be maximized. Y is considerably affected by the distribution of random variables X and Z since $\frac{k_1 N}{k_{-1}}$ is a constant. Z has the normal distribution $N(\mu_z, \sigma_z^2)$ and the entropy of Z can be given as $H(Z) = ln\big(\sigma_z\sqrt{2\pi e}\big)$. The normal distribution has maximum entropy among all real-valued distributions with specified mean and standard deviation. Therefore, to maximize $H(Y)$ we assume that X is a normally distributed random variable with the distribution $N(\mu_x, \sigma_x^2)$. This makes Y a normally distributed random variable with the distribution $N(\mu_y, \sigma_y^2)$ since the summation of two normal distributions is also a normal distribution. Hence, $H(Y)$ can be maximized since it has the normal distribution. Using the linearity of mean and standard deviation of normal distributions, μ_y and σ_y^2 can be given as a linear function of mean and standard deviation of X and Z as follows

$$\mu_y = \frac{k_1 N}{k_{-1}}\mu_x + \mu_z, \quad \sigma_y^2 = (\frac{k_1 N}{k_{-1}}\sigma_x)^2 + \sigma_z^2 \tag{5}$$

Hence, the entropy of Y, i.e., $H(Y)$, can be given as [15]

$$H(Y) = ln\big(\sigma_y\sqrt{2\pi e}\big) = ln\left(\sqrt{2\pi e\left[(\frac{k_1 N}{k_{-1}}\sigma_x)^2 + \sigma_z^2\right]}\right) \tag{6}$$

Hence, using $H(Y)$ and $H(Z)$, the capacity of the single molecular channel between TN and RN, i.e., C_s, can be expressed as

$$C_s = max\Big(I(X;Y)\Big) = H(Y) - H(Z) = \frac{1}{2}ln\left(1 + \frac{(\frac{k_1 N}{k_{-1}}\sigma_x)^2}{\sigma_z^2}\right) \tag{7}$$

Since X is the molecule emission concentration of TN, the minimum value of X is equal to 0. In any normal distribution, % 99.7 of the observations fall within 3 standard deviations of the mean. Therefore, μ_x and σ_x can be approximated as $\mu_x - 3\sigma_x \approx 0$ and $\sigma_x = \mu_x/3$ can be assumed. Similarly, Y cannot be negative and its minimum value is equal to 0. Therefore, μ_y and σ_y can be approximated as $\mu_y - 3\sigma_y \approx 0$ and $\sigma_y = \mu_y/3$ can be assumed.

Next, we introduce the capacity of a molecular multiple-access channel based on the capacity expression of the single molecular channel given in (7).

3 Capacity of Molecular Multiple-Access Channel

In the molecular multiple-access channel, a number of TNs ($TN_1...TN_n$) communicate with a single RN. Each nanomachine has a self-identifying label[2] and adheres the label to the emitted molecules. This mechanism provides a simple addressing scheme to allow RN to distinguish the molecules emitted by each communicating TN [7]. Here, we also assume that TN_i is located to the distance α_i from RN and transmits molecules A with concentration X_i using the binding and release rate k_{1i} and k_{-1}, respectively. X_i is a random variable with the mean μ_{xi} and the variance σ_{xi}^2.

In [10], a model is proposed to find concentration of bound molecules (delivered molecules) for the case in which different molecules bind to a single kind of receptors with a constant concentration. Using this model introduced in [10], the concentration of molecules emitted by TN_i and bind to the receptors on RN, i.e., B_i, can be given as

$$B_i = \frac{\frac{X_i N k_{1i}}{k_{-1}}}{1 + \sum_{j \neq i}^{n} \frac{\mu_{xj} k_{1j}}{k_{-1}}} \tag{8}$$

where N is the concentration of the receptors on RN. Similar to the single molecular channel, we assume that the molecules emitted by TN_i and bind to the receptors on RN, i.e., B_i is exposed to a noise level denoted by Z_i. Thus, the concentration of the bound molecules delivered by TN_i, i.e., Y_i, can be expressed as

$$Y_i = B_i + Z_i = \frac{\frac{X_i N k_{1i}}{k_{-1}}}{1 + \sum_{j \neq i}^{n} \frac{\mu_{xj} k_{1j}}{k_{-1}}} + Z_i, \quad i = 1, ..., n \tag{9}$$

where Z_i is a normally distributed random variable with distribution $N(\mu_{zi}, \sigma_{zi}^2)$ and has the entropy $H(Z_i) = ln\big(\sigma_{zi}\sqrt{2\pi e}\big)$. Similar to the single molecular channel, in order to maximize the entropy of Y_i $(H(Y_i))$, the emitted concentration X_i should have a normal distribution such that this maximization provides the maximum of mutual information $I(X_i; Y_i)$ so as to provide the capacity of the multiple-access channel between TN_i and RN. Therefore, to obtain the capacity, we assume that X_i is a normally distributed random variable with the distribution $N(\mu_{xi}, \sigma_{xi}^2)$. Using the linearity of mean and standard deviation of normal distributions, the mean μ_{yi} and the variance σ_{yi}^2 of the delivered bound molecules (Y_i) can be expressed as

$$\mu_{yi} = \frac{\frac{N k_{1i}}{k_{-1}} \mu_{xi}}{1 + \sum_{j \neq i}^{n} \frac{\mu_{xj} k_{1j}}{k_{-1}}} + \mu_{zi}, \quad \sigma_{yi}^2 = \Big(\frac{\frac{N k_{1i}}{k_{-1}} \sigma_{xi}}{1 + \sum_{j \neq i}^{n} \frac{\mu_{xj} k_{1j}}{k_{-1}}}\Big)^2 + \sigma_{zi}^2 \tag{10}$$

[2] To experimentally investigate the ligand-receptor interactions, three kinds of labeling process called as radio, enzymatic, and fluorescent labeling are mainly used [14]. Here, we assume that each nanomachine has self-identifying labeled molecules used for the molecular communication.

Using σ_{yi}^2, the entropy of Y_i, i.e., $H(Y_i)$, can be given as [15]

$$H(Y_i) = ln(\sigma_{yi}\sqrt{2\pi e}) = ln\left(\sqrt{2\pi e\left[\frac{\frac{Nk_{1i}}{k_{-1}}\sigma_{xi}}{1+\sum_{j\neq i}^{n}\frac{\mu_{xj}k_{1j}}{k_{-1}}}\right]^2+\sigma_{zi}^2}\right) \tag{11}$$

Hence, the capacity of the multiple-access channel between TN_i and RN, i.e., C_{mi}, can be given as

$$C_{mi} = max\Big(I(X_i;Y_i)\Big) = H(Y_i) - H(Z_i) \tag{12}$$

$$C_{mi} = \frac{1}{2}ln\left(1+\frac{\left[\frac{\frac{Nk_{1i}}{k_{-1}}\sigma_{xi}}{1+\sum_{j\neq i}^{n}\frac{\mu_{xj}k_{1j}}{k_{-1}}}\right]^2}{\sigma_{zi}^2}\right) \tag{13}$$

Thus, the capacity of the molecular multiple-access channel, i.e., C_m, can be given as the summation of the capacities achieved by each TN_i as follows

$$C_m = \sum_{i=1}^{n} C_{mi} \tag{14}$$

4 Numerical Results

In this section, we present the numerical analysis on the single and multiple-access molecular channels. The aim of this analysis is to determine the molecular channel characteristics in the single and multiple-access cases. We also aim to observe the changes in these characteristics according to the molecular communication parameters such as number of nanomachines contending on the molecular channels, receptor concentration R, binding rate k_1, and standard deviation of the noise σ_z on the molecular channels. We perform the numerical analysis using Matlab. We assume that TNs and RN are randomly positioned in an spherical shaped environment with radius r_∞, which may have different diffusion coefficients such that it allows TNs to achieve different binding rates (k_1). Moreover, we assume that k_{-1} depends only on the properties of RN receptors and cannot be changed. The simulation parameters of the analysis are given in Table 1.

4.1 Single Molecular Channel

We first observe the effect of the standard deviation of the noise (σ_z) on the capacity of the single molecular channel capacity C_s given in (7). In Fig. 1, the capacity of the single molecular channel (C_s) is shown with the varying standard

Table 1. Simulation Parameters

Binding rate (k_1)	0.1-0.4
Release rate (k_{-1})	0.08
Number of nanomachines (n)	$1-20$
Receptor concentration (N)	$0.01-1$ $(\mu mol/liter)$
Mean of molecule concentration (μ_x)	1-5 $(\mu mol/liter)$
Standard deviation of the noise (σ_z)	0.1-1 $(\mu mol/liter)$

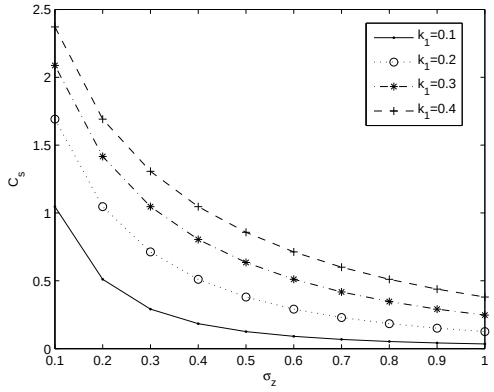


Fig. 1. C_s is shown with varying σ_z for different k_1.

deviation of the noise (σ_z) for different binding rates (k_1). Similar to a wireless communication channel, as the standard deviation of the noise increases, the capacity of single molecular channel decreases. However, the capacity can be improved if higher k_1 can be achieved in the channel. As introduced in (2), the binding rate k_1 is affected by several parameters such as diffusion coefficient of the emitted molecules, size of the environment and nanomachines, and the distance between the nanomachines. These parameters are specific to either the physical properties of the environment or the set up of the network topology in terms of the distance between the nanomachines. Therefore, it may not be possible for TN to increase the binding rate k_1 to improve the single molecular channel capacity despite the increasing noise level. However, it can be possible for TN to increase the mean of the emitted molecule concentration (μ_x) to improve the single molecular channel capacity C_s. In Fig. 2, C_s is shown with varying μ_x for different σ_z. As μ_x increases, C_s can be improved despite the increasing noise level (σ_z).

4.2 Molecular Multiple-Access Channel

We observe the effect of the number of TNs (n), transmitting the molecular information to a single RN, on the capacity of the molecular multiple-access channel capacities C_{mi} given in (13). We assume that a number of TNs are

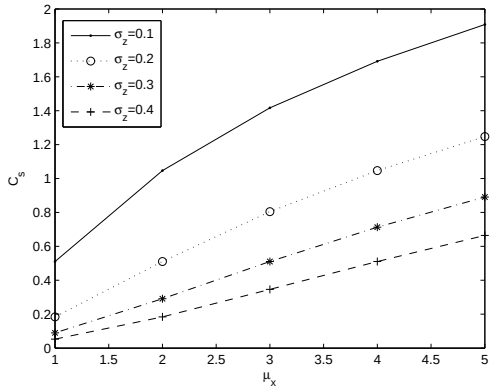
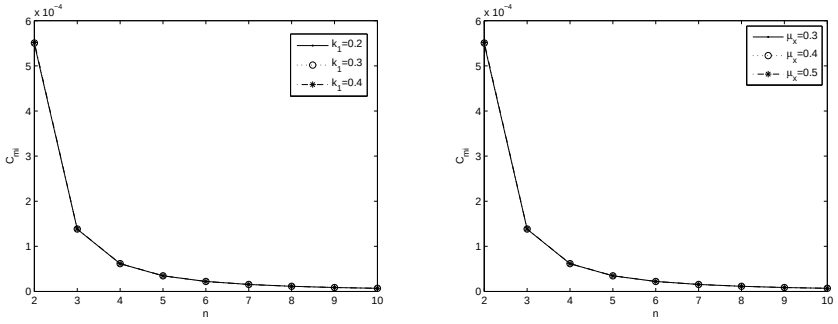


Fig. 2. C_s is shown with varying μ_x for different σ_z.

located around the RN and all of them have the same binding rate k_1 ($k_{1i} = k_1$), the same release rate k_{-1}, and the mean of the emitted molecule concentrations μ_{xi} $\forall i$ are the same for all TNs such that $\mu_{xi} = \mu_x$.



(a) (b)

Fig. 3. (a) C_{mi} is shown with varying n for different k_1. (b) C_{mi} is shown with varying n for different μ_x.

In Fig. 3.a, the molecular communication capacity achieved by a TN in the molecular multiple-access channel, i.e., C_{mi}, is shown with varying number of TNs (n) for different binding rate k_1. In molecular multiple-access channel, due to the contention among TNs to capture the receptors on RN, molecular communication capacity severely reduces with respect to single molecular communication channel on the order of 10^{-4}. C_{mi} also decreases with the number of TNs. Furthermore, contrary to the single molecular channel, as k_1 increases for all TNs contending on the channel, C_{mi} cannot be improved because the excessive contention with the increasing k_1 cannot be mitigated by TNs. Due to the

similar reason based on the increasing contention on the channel, as the mean of the emitted molecules (μ_x) increase, C_{mi} cannot also improved as shown in Fig. 3.b. However, the contention on the molecular multiple-access channel can be mitigated by increasing the receptor concentration (N) on the RN and this way, C_{mi} can be improved. In Fig. 4, C_{mi} is shown with varying n for different receptor concentration on RN. Despite the increasing number of TNs and the excessive contention on the channel, C_{mi} can be improved by increasing the receptor concentration on RN. Thus, an appropriate receptor concentration on RN should be selected according to the contending number of TNs to enable each TN to achieve a satisfactorily high molecular communication capacity.

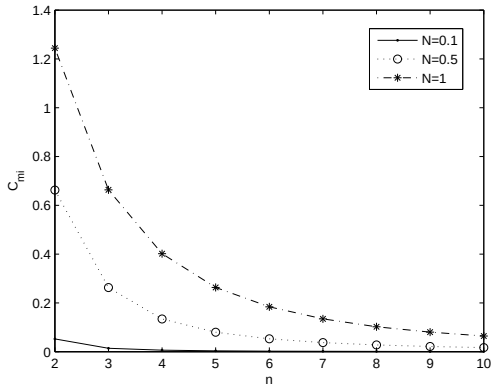


Fig. 4. C_{mi} is shown with varying n for different N.

5 Conclusion

In this paper, we investigate capacity of single and multiple-access molecular channels. We first model these channels similar to Gaussian channel using the principles of natural ligand-receptor binding mechanisms in biology. We then derive the capacity expressions for these channels. Numerical results reveal that high molecular communication capacity can be attainable when molecular communication parameters of nanomachines can be regulated and set. Therefore, efficient molecular communication techniques are essential to efficiently regulate the molecular communication parameters to enable the nanomachines to reliably share the molecular information over the molecular nanonetwork. Based on the theoretical analysis and results in this paper, our ongoing works aim to develop an efficient medium-access and a routing algorithms to provide reliable and effective molecular communication in molecular nanonetworks.

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References

1. Hiyama S., Moritani Y., Suda T., Egashira R., Enomoto A., Moore M., Nakano T.: Molecular Communication. In: Proc. of NSTI Nanotechnology Conference and Trade Show, pp. 391–394, California, USA, (2005)
2. Akyildiz I. F., Brunetti F., Blazquez C.: NanoNetworking: A New Communication Paradigm. Computer Networks (Elsevier), vol. 52, no. 12, pp. 2260–2279, (2008)
3. Moore M., Enomoto A., Nakano T., Egashira R., Suda T., Kayasuga A., Kojima H., Sakakibara H., Oiwa K.: A Design of a Molecular Communication System for Nanomachines Using Molecular Motors. In: Proc. of IEEE International Workshops on Pervasive Computing and Communications (PERCOMW), Italy, (2006)
4. Eckford A. W.: Molecular communication: Physically realistic models and achievable information rates. Submitted to IEEE Transactions on Information Theory, (2008)
5. Eckford A. W.: Nanoscale communication with Brownian motion. In: Proc. of International Conference on Information Sciences and Systems, Baltimore, MD, pp. 160–165, (2007)
6. Atakan B., Akan O. B.: On Channel Capacity and Error Compensation in Molecular Communication. Springer Trans. on Computational System Biology, vol. 10, pp. 59–80, (2008)
7. Atakan B., Akan O. B.: On Molecular Multiple-Access, Broadcast and Relay Channels in Nanonetworks. In: Proc. of ACM International Conference on Bio-Inspired Models of Network, Information, and Computing Systems (BIONETICS), Hyogo, Japan, (2008)
8. Rospars J. P., Krivan V., Lansky P.: Perireceptor and receptor events in olfaction. Comparison of concentration and flux detectors: a modeling study. Chemical Sense, vol. 25, pp. 293–311, (2000)
9. Krivan V., Lansky P., Rospars J. P.: Coding of periodic pulse stimulation in chemoreceptors. Biosystem (Elsevier), vol. 67, pp. 121–128, (2002)
10. Malaka R., Ragg T., Hammer M.: Kinetic models of odor transduction implemented as artificial neural networks. Biological Cybernetics, vol. 73, pp. 195–207, (1995)
11. Northrup S. H., Allison S. A., McCammon J. A.: Brownian dynamics simulation of diffusion-influenced bimolecular reactions. Journal of Chemical Physics, vol. 80, pp. 1517–1524, (1984)
12. Berg H. C., Purcell E. M.: Physics of chemoreception. Biophysical Journal, vol. 20, pp. 193–219, (1977)
13. Chang K. C., Hammer D. A.: The Forward Rate of Binding of Surface-Tethered Reactants: Effect of Relative Motion between Two Surfaces, Biophysical Journal, vol. 76, pp. 1280–1292, (1999)
14. Cooper M. A.: Label-free screening of bio-molecular interactions. Analytical and Bioanalytical Chemistry, vol. 377, pp. 834–842, (2003)
15. Cover T. M., Thomas J. A.: Elements of Information Theory. John Wiley-Sons, (2006)