

Optimal Transmission Probability in Binary Molecular Communication

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Abstract—Molecular communication (MC) is a promising nanoscale communication paradigm that enables nanomachines to share information by using messenger molecules. In this paper, an expression for the achievable rate in MC is first given. Then, using this expression, an optimal transmission probability is developed to maximize the MC rate. Numerical results show that the MC rate is time-dependent and the molecules freely wandering in the medium negatively affect the MC performance. However, the proposed optimal transmission probability is shown to maximize the MC rate.

Index Terms—Molecular communications, nanonetworks, achievable rate, optimal transmission.

I. INTRODUCTION

RAPID development in nano and biotechnology currently paves the way for the fabrication of the nanoscale machines called NanoMachines (NMs). NMs have great potential to provide many promising applications in medicine and industry. However, the realization of these applications is severely prone to uncontrollability and instability problems due to very tiny sizes and unknown physics of NMs. Nevertheless, these problems can be addressed by coordinating NMs via a nanoscale communication. This forms a nanonetwork of NMs and can coordinate different NM populations to reach a sophisticated behavior and to increase the number of design possibilities. Molecular communication (MC) in which molecules are used to share information is one of the most promising paradigms for the realization of nanonetworks [1].

The nanonetworks with MC are conceptualized in [1] and [2]. Besides these initial works, achievable MC rate is investigated [3]–[7]. The molecular noise in the MC channel is also broadly investigated and modeled in [8]. A rigorous stochastic analysis of MC and a noise model for MC are also presented in [9]. The deterministic capacity of molecular information flow in a nanonetwork is explored and the necessity of networking techniques for the realization of future nanonetworks is also discussed in [10]. There are also more recent works on the capacity of molecular communication. In [11], communication capacity is comprehensively investigated for a diffusion-based molecular communication system by taking into account the channel memory and molecular noise. A channel model and capacity analysis are also given in [12] for the case in which the messenger molecules have 1-D motion and they may degrade. In [13], a molecular relay channel is analyzed to find out its communication capacity. The performance of the active molecular communication in microchannels is also

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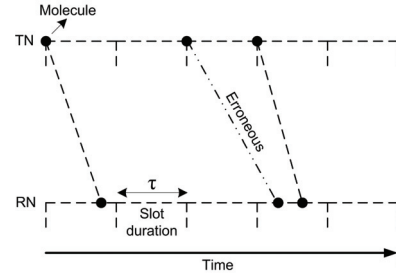


Fig. 1. A timing diagram of the MC between TN and RN.

explored in [14]. Furthermore, the recent survey papers [15]–[17] extensively overview the current literature of molecular communication.

In this paper, an expression is derived for MC rate. Then, based on this expression an optimal transmission probability is derived to ensure the maximum achievable MC rate. Next, a MC model and a rate expression for MC are introduced in Section II. An optimal transmission probability is derived in Section III. Finally, numerical results and concluding remarks are presented in Section IV and V.

II. BINARY MOLECULAR COMMUNICATION MODEL

In this paper, a binary MC scheme is considered. In order to transmit bit 1, the Transmitter Nanomachine (TN) emits a molecule at the beginning of the slot duration¹, i.e., τ . The bit 1 is assumed to be successfully delivered if the Receiver Nanomachine (RN) receives the molecule during τ . For the transmission of bit 0, TN emits no molecule and it is assumed to be successfully delivered if RN does not receive any molecule during τ . Otherwise, the current transmission attempt becomes unsuccessful. In Fig. 1, a timing diagram for the defined binary MC scheme is illustrated. The movement of molecules is assumed to be governed by a Brownian motion. Then, the delay t experienced by any molecule to reach RN obeys the following probability density function [19].

$$f(t) = \frac{d}{\sqrt{4\pi Dt^3}} e^{-\frac{d^2}{4Dt}}, \quad t > 0 \quad (1)$$

where D is the diffusion coefficient of the molecules and d is the Euclidean distance between TN and RN. Notice that $f(t)$ characterizes the delay for one dimensional motion of molecules. However, all analyses given in the rest of the paper are directly applicable to two and three dimensional motion with appropriate probability density functions. The cumulative

¹Here, the nanomachines are assumed to synchronize with each other to emit and receive each molecule within the fixed duration time slots. Note that synchronization of nanomachines has been already investigated in the literature. For example, in [18], the oscillatory behavior of individual cells can be synchronized via inter-cell signaling.

distribution function associated with the density function $f(t)$ in (1), i.e., $F(t)$, can be given as

$$F(t) = \text{Erfc}\left(\frac{d}{2\sqrt{Dt}}\right), \quad t > 0. \quad (2)$$

Let assume that TN transmits 1 at slot n with the probability β_n or transmits 0 with the probability $(1 - \beta_n)$. Hence, the channel input at slot n , i.e., X_n , can be characterized as $X_n \sim \text{Bernoulli}(\beta_n)$, $\forall n \in \{1, 2, \dots\}$. If the molecule emitted at slot n is just taken into account, the following probabilities can be derived. For the case of $X_n = 1$, the probability that RN successfully receives 1, i.e., α_n , can be given as $\alpha_n = \beta_n F(\tau)$. However, the probability that the emitted molecule fails to reach RN and 1 cannot be successfully received within slot n , i.e., ξ_n , is $\xi_n = \beta_n (1 - F(\tau))$. In this case, RN erroneously receives 0 instead of 1. Furthermore, if TN emits no molecule at slot n , which means $X_n = 0$, the probability that RN successfully receives 0, i.e., ζ_n , can be expressed as $\zeta_n = (1 - \beta_n)$. Consequently, if the molecule emitted at slot n is just taken into account, RN receives 1 with α_n and receives 0 with $\xi_n + \zeta_n = (1 - \alpha_n)$ during slot n . This can be also characterized by a Bernoulli random variable, i.e., $G_n \sim \text{Bernoulli}(\alpha_n)$.

In addition to the molecule emitted at slot n , RN may also receive the molecules that have been transmitted for the previous $n - 1$ slot duration and have not been received by RN. Suppose that a molecule, that is emitted at slot k with probability β_k and has not been received by RN. Note that $k \in \{1, 2, \dots, n - 1\}$. Clearly, this molecule may be received by RN at slot n since every emitted molecule continuously diffuses in the medium until it is received by RN. In such a case, the probability that the molecule, emitted at slot k , is received at slot n , i.e., λ_{nk} , can be given as

$$\lambda_{nk} = \beta_k \left[F((n - k + 1)\tau) - F((n - k)\tau) \right], \quad k < n \quad (3)$$

Notice that λ_{nk} is only available for $k < n$. Furthermore, the probability that the molecule emitted at slot k is not received by RN during slot n is $(1 - \lambda_{nk})$. In fact, such a late molecule can be considered as a noise of the channel and its effect on the channel, i.e., $\Gamma_{n,k}$, can be characterized by a Bernoulli random variable, that is, $\Gamma_{n,k} \sim \text{Bernoulli}(\lambda_{nk})$. Similar to slot k , each noise term coming from previous $(n - 1)$ slots can be modeled as a Bernoulli random variable, i.e., $\Gamma_{n,k} \sim \text{Bernoulli}(\lambda_{nk})$, $\forall k \in \{1, 2, \dots, n - 1\}$. Hence, by adding all of these noise terms, total noise at slot n , i.e., Z_n , can be expressed as

$$Z_n = \sum_{k=1}^{n-1} \Gamma_{n,k} \quad (4)$$

Here, note that each $\Gamma_{n,k}$ is independent of each other since each of them depends on a different channel transmission probability β_k , $k \in \{1, \dots, n - 1\}$. Furthermore, $\Gamma_{n,k}, \forall k$ are independent from G_n since G_n only depends on β_n while $\Gamma_{n,k}, \forall k$ do not depend on β_n . By considering $G_n \sim \text{Bernoulli}(\beta_n F(\tau))$ and Z_n , the channel output at slot n , i.e., Y_n , can be given as $Y_n = G_n + Z_n$. Here, the channel output, Y_n , and noise, Z_n , are the sum of Bernoulli random variables with ranges $\{0, 1, 2, \dots, n\}$ and $\{0, 1, 2, \dots, n - 1\}$,

respectively. Thus, they can be characterized by two *Poisson-Binomial* random variables. Using the probability λ_{nk} in (3), the Probability Mass Functions (PMFs) of Y_n and Z_n can be respectively given as

$$p_i = \sum_{A \in \mathcal{S}_i} \prod_{k \in A} \lambda_{nk} \prod_{j \in A^c} (1 - \lambda_{nj}) \quad (5)$$

$$q_i = \sum_{B \in \mathcal{T}_i} \prod_{l \in B} \lambda_{nl} \prod_{m \in B^c} (1 - \lambda_{nm}) \quad (6)$$

where p_i and q_i are the point probabilities of Y_n and Z_n , that is, $\text{Pr}(Y_n = i) = p_i, i \in \{0, 1, \dots, n\}$ and $\text{Pr}(Z_n = i) = q_i, i \in \{0, 1, \dots, n - 1\}$. \mathcal{S}_i and \mathcal{T}_i are the sets that include all subsets of i integers that can be selected from $\{1, 2, \dots, n\}$ and $\{1, 2, \dots, n - 1\}$, respectively. For example, if $n = 3$, then i is selected from $\{1, 2, 3\}$ to form \mathcal{S}_i and selected from $\{1, 2\}$ to form \mathcal{T}_i . In this case, \mathcal{S}_2 and \mathcal{T}_2 can be given as $\mathcal{S}_2 = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$ and $\mathcal{T}_2 = \{\{1, 2\}\}$. A denotes the elements of \mathcal{S}_i and A^c is the complement of A , i.e., $A^c = \{1, 2, \dots, n\} \setminus A$. Furthermore, B denotes an element of \mathcal{T}_i and B^c is the complement of B .

The mutual information between the channel input $X_n \sim \text{Bernoulli}(\beta_n)$ and the output Y_n with the PMF given in (5) can be expressed as

$$\begin{aligned} I(X_n; Y_n) &= H(Y_n) - H(Y_n | X_n) \\ &= H(G_n + Z_n) - H(G_n + Z_n | X_n) \end{aligned} \quad (7)$$

Since $X_n \sim \text{Bernoulli}(\beta_n)$ and $G_n \sim \text{Bernoulli}(\beta_n F(\tau))$ and $F(\tau)$ is a constant probability, G_n can be determined if X_n is given. Furthermore, X_n and Z_n are independent. Thus, $H(G_n | X_n) = 0$ and $H(Z_n | X_n) = H(Z_n)$ and using p_i and q_i in (5) and (6), $I(X_n; Y_n)$ can be written as

$$\begin{aligned} I(X_n; Y_n) &= H(Y_n) - H(Z_n) \\ &= - \sum_{i=0}^n p_i \log p_i + \sum_{i=0}^{n-1} q_i \log q_i \end{aligned} \quad (8)$$

Note that each noise term in (4) can be considered as the effect of channel memory. These effects are summarized in Z_n to obtain an approximation for the maximum achievable MC rate. Hence, $I(X_n; Y_n)$ can be considered as $\frac{1}{n} I(X_1, X_2, \dots, X_n; Y_1, Y_2, \dots, Y_n)$. Next, a close-form expression is derived for the optimal value of β_n which maximizes $I(X_n; Y_n)$ to obtain the maximum achievable rate during the slot n .

III. OPTIMAL TRANSMISSION PROBABILITY IN MC

In this section, a tight approximation for the optimal β_n is provided to maximize $I(X_n; Y_n)$. To this end, using the statistical dependence between p_i and q_i given in (5) and (6), p_i can be first expressed as a function of q_i and α_n as follows.

$$\begin{aligned} p_i &= \alpha_n q_{i-1} + (1 - \alpha_n) q_i \\ &= q_i + \alpha_n (q_{i-1} - q_i) \\ &= q_i + \beta_n F(\tau) (q_{i-1} - q_i) \\ &= q_i + \beta_n F(\tau) r_i \end{aligned} \quad (9)$$

where $r_i = q_{i-1} - q_i$. By substituting $p_i = q_i + \beta_n F(\tau) r_i$ into $I_n(X_n; Y_n)$, $\frac{\partial I_n}{\partial \beta_n}$ can be written as

$$\frac{\partial I_n}{\partial \beta_n} = - \sum_{i=0}^n F(\tau) r_i \log [q_i + \beta_n F(\tau) r_i] - \sum_{i=0}^n F(\tau) r_i \quad (10)$$

Note that I_n is hereafter used to denote $I(X_n; Y_n)$. Since q_{-1} and q_n are equal to 0, $\sum_{i=0}^n F(\tau) r_i = F(\tau)(q_{-1} - q_0 + q_0 - q_1 + q_1 - q_2 + \dots - q_{n-1} + q_{n-1} - q_n) = 0$. Then, (10) can be given as

$$\begin{aligned} \frac{\partial I_n}{\partial \beta_n} &= -F(\tau) r_0 \log [q_0 + \beta_n F(\tau) r_0] - \\ &- \sum_{i=1}^n F(\tau) r_i \log \left[\left[1 + \frac{q_i}{\beta_n F(\tau) r_i} \right] \beta_n F(\tau) r_i \right] \end{aligned} \quad (11)$$

For the solution of $\frac{\partial I_n}{\partial \beta_n} = 0$, the approximation, $\log(1+x) \approx x$ for $|x| < 0.1$, can be applied to $\log \left[1 + \frac{q_i}{\beta_n F(\tau) r_i} \right]$ in (11) for $\left| \frac{q_i}{\beta_n F(\tau) r_i} \right| < 0.1 \forall i$ and this yields

$$\begin{aligned} \frac{\partial I_n}{\partial \beta_n} &\approx -F(\tau) r_0 \log [q_0 + \beta_n F(\tau) r_0] - \\ &- \sum_{i=1}^n F(\tau) r_i \left[\log [F(\tau) r_i] + \log[\beta_n] \right] - \sum_{i=1}^n \frac{q_i}{\beta_n} \end{aligned} \quad (12)$$

Due to $\sum_{i=1}^n r_i = q_0$, $\sum_{i=1}^n q_i = 1 - q_0$, and $r_0 = -q_0$, (12) can be also modified as

$$\begin{aligned} \frac{\partial I_n}{\partial \beta_n} &\approx -F(\tau) q_0 \left[\log \left(1 + \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right) \right] - \\ &\frac{(1 - q_0)}{\beta_n} - \sum_{i=1}^n F(\tau) r_i \log [F(\tau) r_i] - F(\tau) q_0 \log \left[\frac{1}{q_0} \right] \end{aligned} \quad (13)$$

In (13), $\log \left(1 + \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right)$ can be approximated as $\frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)}$ for $\left| \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right| < 0.1$ and substituting this approximation into (13),

$$\begin{aligned} \frac{\partial I_n}{\partial \beta_n} &\approx -F(\tau) q_0 \left[\frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right] - \frac{(1 - q_0)}{\beta_n} \\ &- \sum_{i=1}^n F(\tau) r_i \log [F(\tau) r_i] - F(\tau) q_0 \log \left[\frac{1}{q_0} \right] \end{aligned} \quad (14)$$

can be obtained. Finally, solving $\frac{\partial I_n}{\partial \beta_n} = 0$ in (14), the optimal β_n , i.e., $\hat{\beta}_n$, can be given as in (18). In (18), δ is

$$\delta = \sum_{i=1}^n F(\tau) r_i \log F(\tau) r_i - F(\tau) q_0 \log(q_0) \quad (15)$$

Since $\log(1+x) \approx x$ is tight for $|x| < 0.1$, the tightness of the approximations in (12) and (14) also requires to satisfy the following two conditions, i.e., cmd_1 and cmd_2 :

$$cmd_1 = \left| \frac{q_i}{\beta_n F(\tau) r_i} \right| < 0.1, \forall i \in \{1, \dots, n-1\} \quad (16)$$

$$cmd_2 = \left| \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right| < 0.1 \quad (17)$$

In Section IV, these conditions, cmd_1 and cmd_2 , are numerically evaluated for the tightness of the approximations. As observed in (18), the optimal value of β_n , i.e. $\hat{\beta}_n$, is a function of $F(\tau)$ and q_i , $i \in \{0, \dots, n-1\}$. Hence, it is possible to

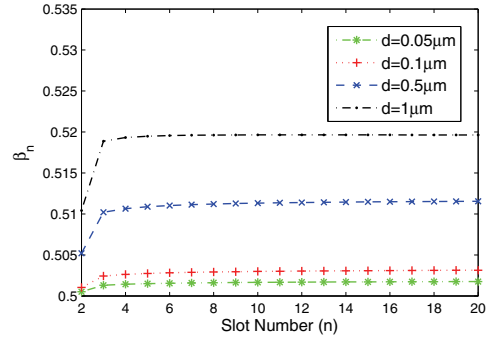


Fig. 2. $\hat{\beta}_n$ with varying slot number for the different distance values, i.e., d , between TN and RN.

iteratively compute $\hat{\beta}_n$ for each slot n . For example, at slot 10, $\hat{\beta}_{10}$ can be computed by using $F(\tau)$ and q_i , $i = \{0, \dots, 9\}$. For this, an arbitrary β_1 is initially selected, then, $\hat{\beta}_2$ are found by computing q_0 and q_1 and substituting them into (18) and (15). Similarly, each β_n , $n \in \{2, \dots\}$ can be consecutively computed by using $\beta_1, \hat{\beta}_2, \dots, \beta_{n-1}$. Next, we present the numerical results on the maximum MC rate and $\hat{\beta}_n$.

IV. NUMERICAL RESULTS

In this section, the numerical results on the optimal transmission probability, $\hat{\beta}_n$, in (18) and the maximum achievable MC rate obtained by using $\hat{\beta}_n$ are presented for varying system parameters. TN is assumed to emit molecules by starting from slot 1. Furthermore, β_1 is set to $\beta_1 = 0.3$ and τ is set to $\tau = 0.5s$ throughout the numerical evaluations. In Fig. 2, $\hat{\beta}_n$ is shown as the slot number changes from 1 to 20 for different distance values, i.e., d , between TN and RN. For all d values ranging from $d = 0.05 \mu m$ to $d = 1 \mu m$, $\hat{\beta}_n$ slightly increases with d and quickly converges to the optimal values rather than oscillating around some specific values. This can make the determination of the efficient channel codes feasible. The convergent $\hat{\beta}_n$ is used to determine the average number of bits 1 in the code words to ensure high MC rate. For the same setting used in Fig. 2, maximum achievable MC rate, i.e., C_n , is shown in Fig. 3. Note that C_n values in Fig. 3 are computed by using $\hat{\beta}_n$ values in Fig. 2. The maximum achievable MC rate grows from 0.61 to 0.69 *nats/trans.* or from 0.88 to 0.993 *bits/trans.* at slot 20 as TN and RN become close to each other. This reveals that the optimal transmission probability provides a very high molecular communication rate up to 0.993 *bits/trans.*. Furthermore, C_n reduces as the slot number proceeds and this reduction becomes higher as d increases because the diffusing molecules negatively affect the MC performance. However, this decrease in C_n requires a rigorous convergence analysis to determine the lower-bound of the rate. Furthermore, in order to show the tightness of the $\hat{\beta}_n$ computation in Fig. 2, the conditions cmd_1 and cmd_2 are shown in Fig. 4 and 5, respectively. Since $|cmd_1| < 0.1$ and $|cmd_2| < 0.1$ can be always satisfied as observed in the figures, the computed $\hat{\beta}_n$ values are the tight approximations to the optimal values of the channel transmission probability β_n .

$$\hat{\beta}_n \approx \frac{-\delta + F(\tau) - \sqrt{[\delta - F(\tau)]^2 - 4(1 - q_0) [-\delta F(\tau) + F(\tau)q_0 + F(\tau)^2 q_0]}}{2 [-\delta F(\tau) + F(\tau)q_0 + F(\tau)^2 q_0]} \quad (18)$$

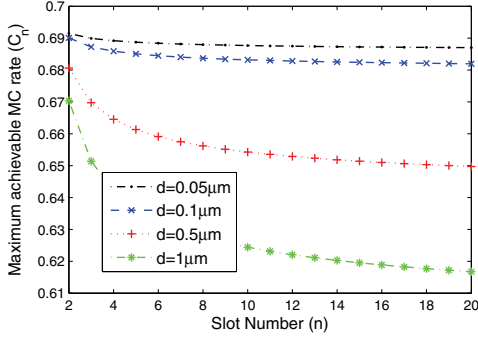


Fig. 3. The maximum achievable MC rate, i.e., C_n , with varying slot number for the different values of d .

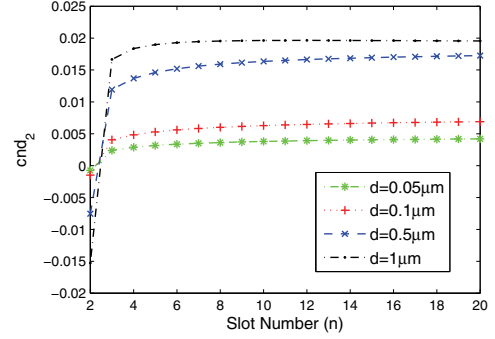


Fig. 5. cnd_2 with varying slot number for the different values of d .

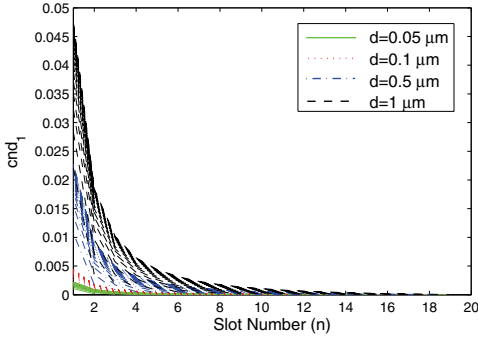


Fig. 4. cnd_1 with varying slot number for the different d values.

V. CONCLUSION

In this paper, a rate expression for molecular communication are first developed. Then, an optimal transmission probability is derived to reach the maximum achievable MC rate. The results reveal that the freely wandering molecules negatively affect the MC rate. However, the proposed optimal transmission probability can maximize the MC rate by taking into account all emitted molecules.

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