Enabling Energy Efficient Molecular Communication via Molecule Energy Transfer

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***Abstract*—Molecular communication via diffusion (MCvD) is inherently an energy efficient transportation paradigm, which requires no external energy during molecule propagation. Inspired by the fact that the emitted molecules have a finite probability to reach the receiver, this paper introduces an energy efficient scheme for the information molecule synthesis process of MCvD via a simultaneous molecular information and energy transfer (SMIET) relay. With this SMIET capability, the relay can decode the received information as well as generate its emission molecules using its absorbed molecules via chemical reactions. To reveal the advantages of SMIET, approximate closed-form expressions for the bit error probability and the synthesis cost of this two-hop molecular communication system are derived and then validated by particle-based simulation. Interestingly, by comparing with a conventional relay system, the SMIET relay system can be shown to achieve a lower minimum bit error probability via molecule division, and a lower synthesis cost via molecule type conversion or molecule division.**

***Index Terms*—Molecular communication, energy transfer, chemical reaction, SMIET relay.**

I. Introduction

Recently, molecular communication has been proposed as the potential enabler for nano-scale communication between nanomachines via the transmission of chemical signals in very small dimensions or in specific environments, such as in salt water, tunnels, or human bodies. Among all types of molecular communication paradigms, molecular communication via diffusion (MCvD) allows the information molecules to propagate freely via random Brownian motion, and it is the most simple, general and energy efficient transportation paradigm, since it does not require external energy or infrastructure.

Even though the propagation of information molecules in MCvD does not need external energy, molecule synthesis at the transmitter is energy consuming, and currently nano-batteries for nanomachines do not exist. Moreover, supplying power externally via acoustic or electromagnetic waves to nanomachines operating in vivo can be difficult due to high penetration loss and its small dimensions. Hence, how to reduce the molecule synthesis cost to improve energy efficiency in molecular communication becomes an important question to answer.

One way to reduce the synthesis cost is to collect the information molecules arriving at the nanomachine not only for received signal decoding, but also for its own information transmission use. This process is the so called simultaneous molecular information and energy transfer (SMIET) process [1]. In fact, SMIET-like processes can be found at the cellular level in biology; one example is the γ-Aminobutyric acid (GABA) metabolism and uptake, which is usually found in all regions of the mammalian brain [2]. In this mechanism, GABA, which is generated and released by the presynaptic neuron cell (i.e., source), can be harvested and converted to Glutamine inside the neighbouring Glial cells (i.e., SMIET relay) for further transmission. The SMIET process can also be engineered in a cell by using genetic circuits with chemical reactions facilitated by catalysts [3].

To construct an energy efficient system, we propose and study a two-hop molecular communication system with an absorbing SMIET relay, where the relay has the capability of converting the absorbed molecules to another type of molecule via chemical reactions for its own transmission to save its synthesis cost. To showcase the benefits of the proposed system, we derive closed-form expressions for the approximate bit error probability at the destination and the system synthesis cost. These are verified by particle-based simulations. Our results show that with the help of the SMIET relay in the two-hop molecular communication system, the minimum bit error probability can be greatly improved, whereas the synthesis cost with molecule type conversion and that with molecule division are reduced compared to that of a conventional relay system.

II. System Model

We propose a two-hop SMIET molecular communication system with a point source, an absorbing decode-and-forward (DF) relay with radius R_R, and an absorbing destination with radius R_D. Here, we limit ourselves to the full absorption receiver case as in [4], which can be extended to the partial absorption receiver [4]. In this two-hop SMIET molecular communication system, the relay can absorb the type A molecules transmitted by the source located at a distance d_R away from the surface of the relay. With the absorbed type A molecules, the relay operates in SMIET mode to decode the information as well as to convert type A molecules to type B molecules, then the relay transmitter emits the generated type B molecules for the intended destination at a distance d_D away from the surface of the destination.

The type A information molecule and the type B information molecule are molecules with an arbitrary shape and effective radius r_A and r_B ($r_A, r_B \ll R_R, R_D$), respectively. We assume that $r_A = lr_B, (l > 0)$. The diffusion coefficient is generally inversely proportional to the radius [5], [6], thus we have the diffusion coefficient of type A molecule D_A and the diffusion coefficient of type B molecule D_B following the relationship $D_B = lD_A$. We

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assume that the relay has specific receptors that only absorb type A molecules transmitted by the source, and the destination has different receptors that only absorb type B molecules transmitted by the relay for information decoding. Otherwise, each receiver is transparent to the non-specific molecule type.

A. Source to Relay Link

In the source to relay link, the source transmits the jth bit at time $t = (j-1)T_b$ by modulating the number of type A molecules with binary concentration shift keying (BCSK), where the source emits N_A type A molecules to transmit bit-1 and emits 0 molecules to transmit bit-0. T_b is the single bit interval time, and $T_b = T_{\rm R} + T_{\rm D}$, where $T_{\rm R}$ and $T_{\rm D}$ are the first hop and second hop time intervals, respectively. As in [7]–[9], we decode using the net number of absorbed molecules in the current interval. Thus, the relay measures the number of absorbed type A molecules $N_{\rm R}^{\rm new}[j]$ during the first hop interval $[(j-1)T_b, (j-1)T_b + T_{\rm R}]$. $N_{\rm R}^{\rm new}[j]$ is used for information decoding of the jth bit and molecular energy transfer and for powering the second hop transmission.

B. SMIET Relay

The SMIET relay receiver is capable of performing division from a type A molecule into one or more type B molecules via a chemical reaction in a short time with the help of a reaction catalyst, and one example is the protein degradation of type A molecule into subunits [10]. We express this reaction as [11]

$$\mathrm{A} \rightarrow m\mathrm{B}, \tag{1}$$

where each absorbed type A molecule is instantaneously decomposed[1] into m type B molecules inside the relay. We idealistically assume that this reaction only occurs during the interval of the *first* hop. However, the implementation of time-varying reaction kinetics is outside the scope of this work.

C. Relay to Destination Link

In the model, a barrel transmitter with negligible radius is located on the surface of the relay. It is placed at the point closest to the destination. We assume that there is no interaction between the type A molecules and the type B molecules outside the relay, due to the lack of catalyst, and transformation of type-A to type-B only occurs inside the relay. The type B molecules transmitted by the relay will not be absorbed by the relay (since the relay only absorbs type A molecules), and the relay can be treated as a point transmitter during the transmission process.

In the relay to destination link, the relay forwards the decoded signal by modulating on the number of converted type B molecules at the relay. If the received signal at the relay $\hat{x}_{\rm R}[j]$ is bit-1, then the relay transmitter emits $mN_{\rm R}^{\rm new}[j]$ type B molecules to the destination at $t = (j-1)T_b + T_{\rm R}$; if the received signal at the relay $\hat{x}_{\rm R}[j]$ is bit-0, then the relay transmitter emits zero molecules. The destination then decodes the signal $\hat{x}_{\rm D}[j]$ based on the net number of type B molecules absorbed at the destination during $[(j-1)T_b + T_{\rm R}, jT_b]$.

[1]Fast enzymatic reactions can occur at timescales of 1 μs or less, which is much faster than the diffusion times considered in Section IV. By assuming instantaneous conversion, the derived error probability is a lower bound and the synthesis cost is an upper bound to that in the finite reaction rate scenario.

III. Error Probability and Synthesis Cost

In this section, we examine the bit error probability and the synthesis cost in the two-hop molecular communication system with the proposed SMIET mechanism.

A. Bit Error Probability at the Relay

For multiple bit transmission, the net number of absorbed type A molecules received at the relay in the jth bit interval can be modeled as [7, Eq. (26)] [12, Eq. (8)]

$$N_{\rm R}^{\rm new}[j] \sim \mathrm{Pois}(N_{\rm A}\Psi_{\rm R}[j]), \tag{2}$$

where

$$\Psi_{\rm R}[j] = \sum_{i=1}^{j} x_{\rm S}[i]\, R\left(d_{\rm R}, r_{\rm R}, D_{\rm A}, (j-i)T_b, (j-i)T_b + T_{\rm R}\right), \tag{3}$$

$$R(d_{\rm R}, r_{\rm R}, D_{\rm A}, T, T+T_{\rm R}) = \frac{r_{\rm R}}{r_{\rm R}+d_{\rm R}} \left[\mathrm{erfc}\left\{\frac{d_{\rm R}}{\sqrt{4D_{\rm A}(T+T_{\rm R})}}\right\} - \mathrm{erfc}\left\{\frac{d_{\rm R}}{\sqrt{4D_{\rm A}T}}\right\}\right], \tag{4}$$

$x_{\rm S}[i]$ is the ith transmitted bit at the source, and Pois is the Poisson distribution. The Poisson approximation is accurate for sufficiently large $N_{\rm A}$ and sufficiently small $\Psi_{\rm R}[j]$.

The received signal at the relay is decoded as follows: if $N_{\rm R}^{\rm new}[j] < N_{\rm th}^{\rm R}$, then the received signal $\hat{x}_{\rm R}$ at the relay is bit-0; otherwise, $\hat{x}_{\rm R}$ is bit-1, where $N_{\rm th}^{\rm R}$ is the decision threshold at the relay. The error probability of the jth bit is

$$\begin{aligned} P_e^{\rm R}[j] =& P_1 P_e^{\rm R}\left[\hat{x}_{\rm R}[j]=0 \,\middle|\, x_{\rm S}[j]=1, x_{\rm S}[1:j-1]\right] \\ &+ P_0 P_e^{\rm R}\left[\hat{x}_{\rm R}[j]=1 \,\middle|\, x_{\rm S}[j]=0, x_{\rm S}[1:j-1]\right], \end{aligned} \tag{5}$$

where

$$\begin{aligned} &P_e^{\rm R}\left[\hat{x}_{\rm R}[j]=0 \,\middle|\, x_{\rm S}[j]=1, x_{\rm S}[1:j-1]\right] \\ &\quad\approx \exp\left\{-N_{\rm A}\Psi_{\rm R}^1[j]\right\} \sum_{n=0}^{N_{\rm th}^{\rm R}-1} \frac{\left[N_{\rm A}\Psi_{\rm R}^1[j]\right]^n}{n!}, \end{aligned} \tag{6}$$

and

$$\begin{aligned} &P_e^{\rm R}\left[\hat{x}_{\rm R}[j]=1 \,\middle|\, x_{\rm S}[j]=0, x_{\rm S}[1:j-1]\right] \\ &\quad\approx 1 - \exp\left\{-N_{\rm A}\Psi_{\rm R}^0[j]\right\} \sum_{n=0}^{N_{\rm th}^{\rm R}-1} \frac{\left[N_{\rm A}\Psi_{\rm R}^0[j]\right]^n}{n!}, \end{aligned} \tag{7}$$

respectively [7, Eqs. (32), (33)]. In (6) and (7), $\Psi_{\rm R}^1[j]$ and $\Psi_{\rm R}^0[j]$ are given in (3) with $x_{\rm S}[j]=1$ and $x_{\rm S}[j]=0$, respectively. In (5), P_1 and P_0 denote the probability of sending bit-1 and bit-0, respectively.

B. Bit Error Probability at the Destination

Each absorbed type A molecule is converted to m type B molecules for transmission at the relay, thus, the net number of absorbed type B molecules received in the jth bit interval during

$[(j-1)T_b + T_{\rm R}, jT_b]$ is described as a binomial distribution

$$N_{\rm D}^{\rm new}[j] \sim \sum_{i=1}^{j} B\Big(mN_{\rm R}^{\rm new}[i], \hat{x}_{\rm R}[i] \times R\left(d_{\rm D}, r_{\rm R}, D_B, (j-i)T_b, (j-i)T_b + T_D\right)\Big), \quad (8)$$

where $\hat{x}_{\rm R}[i]$ is the ith detected bit at the relay.

According to the fact that Y follows a Poisson distribution $Y \sim \text{Pois}(\lambda p)$ when we have the conditional binomial distribution $Y|(X=x) \sim B(x,p)$ and $X \sim \text{Pois}(\lambda)$[2] [14], we approximate $N_{\rm D}^{\rm new}[j]$ as

$$\begin{aligned} N_{\rm D}^{\rm new}[j] &\sim \sum_{i=1}^{j} \text{Pois}\Big(mN_{\rm A}\Psi_{\rm R}[i]\hat{x}_{\rm R}[i] \\ &\quad \times R\left(d_{\rm D}, r_{\rm D}, D_{\rm B}, (j-i)T_b, (j-i)T_b + T_{\rm D}\right)\Big) \\ &\sim \text{Pois}(N_{\rm A}\Psi_{\rm D}[j]), \end{aligned} \quad (9)$$

where

$$\begin{aligned} \Psi_D[j] = \sum_{i=1}^{j} m\Psi_{\rm R}[i]\hat{x}_{\rm R}[i] R\left(d_{\rm D}, r_{\rm D}, D_B, \right. \\ \left. (j-i)T_b, (j-i)T_b + T_{\rm D}\right), \end{aligned} \quad (10)$$

and $\Psi_{\rm R}[i]$ is given in (3). We note that $N_{\rm D}^{\rm new}[j]$ is dependent on constant parameters and the detected signals at the relay, but not on $N_{\rm R}^{\rm new}[i]$.

The destination decodes the received signal by comparing the net number of absorbed molecules in the second hop interval $N_{\rm D}^{\rm new}[j]$ with the destination decision threshold $N_{\rm th}^{D}$. Thus, the error probability of the jth bit at the destination is

$$\begin{aligned} P_e^{\rm D}[j] =& P_1 P_e^{\rm D}\left[\hat{x}_{\rm D}[j] = 0 \left| x_{\rm S}[j] = 1, x_{\rm S}[1:j-1]\right.\right] \\ &+ P_0 P_e^{\rm D}\left[\hat{x}_{\rm D}[j] = 1 \left| x_{\rm S}[j] = 0, x_{\rm S}[1:j-1]\right.\right], \end{aligned} \quad (11)$$

where

$$\begin{aligned} &P_e^{\rm D}\left[\hat{x}_{\rm D}[j] = 0 \left| x_{\rm S}[j] = 1, x_{\rm S}[1:j-1]\right.\right] \\ &= \exp\left\{-N_{\rm A}\Psi_{\rm D}^1[j]\right\} \sum_{n=0}^{N_{\rm th}^{\rm D}-1} \frac{\left[N_D\Psi_{\rm D}^1[j]\right]^n}{n!}, \end{aligned} \quad (12)$$

and

$$\begin{aligned} &P_e^{\rm D}\left[\hat{x}_{\rm D}[j] = 1 \left| x_{\rm S}[j] = 0, x_{\rm S}[1:j-1]\right.\right] \\ &= 1 - \exp\left\{-N_{\rm A}\Psi_{\rm D}^0[j]\right\} \sum_{n=0}^{N_{\rm th}^{\rm D}-1} \frac{\left[N_D\Psi_{\rm D}^0[j]\right]^n}{n!}, \end{aligned} \quad (13)$$

respectively. In (12) and (13), $\Psi_{\rm D}^1[j]$ and $\Psi_{\rm D}^0[j]$ are given in (10) with $x_{\rm S}[j] = 1$ and $x_{\rm S}[j] = 0$, respectively. As can be seen in (10), the bit error probability is a function of the detected bits at the relay $\hat{x}_{\rm R}[1:k]$. To calculate (11) with low computational complexity, we average the bit error probability over many realizations of $\hat{x}_{\rm R}[1:k]$ to obtain an approximation. Each realization of $\hat{x}_{\rm R}[1:k]$ is obtained by tossing a biased coin for each bit. Specifically, given $x_S[k] = \nu_S \in \{0,1\}$, we toss a biased coin to determine whether the detected bit at the relay is $\hat{x}_{\rm R}[k] = x_S[k]$, which occurs with probability equal to $1 - P_e^{\rm R}\left[\hat{x}_{\rm R}[k] = |1-\nu_S| \left| x_{\rm S}[k] = \nu_S, x_{\rm S}[1:j-1]\right.\right]$ given in (6) and (7). Our simulation results in Section IV confirm the accuracy of this approximation.

[2]Here, the approximation $mN_{\rm R}^{\rm new}[j] \sim \text{Pois}(mN_{\rm A}\Psi_{\rm R}[j])$ is obtained from that for the sum of correlated Poisson variables in [13, pp. 63-64].

C. Synthesis Cost at the Source

We now present the energy model for the proposed SMIET relay system. In biological cells, most energy-requiring reactions are powered by the Gibbs free energy released by the hydrolysis of Adenosine triphosphate (ATP) [11]. Thus, ATP is useful in many cell processes, such as photosynthesis, active transport across cell membranes (as in the electron transport chain), and synthesis of macromolecules (e.g., DNA).

To quantify the synthesizing energy cost of the type A molecule and type B molecule, we use the amount of Gibbs free energy G^0 released from hydrolysis of ATP as [11]

$$ATP + H_20 \rightarrow ADP + P_I, \qquad \Delta G^0 = -30.5 \text{ kJ/mol}, \quad (14)$$

where ADP is adenosine diphosphate, and P_I is phosphate. We assume that the synthesis of a single type A molecule requires $g_{\rm A}$ ATPs, and that of single type B molecule requires $g_{\rm B}$ ATPs. As such, the synthesizing energy cost of a single type A molecule, $G_{\rm A}$, and that of a single type B molecule, $G_{\rm B}$, are calculated as

$$G_{\rm A} = g_{\rm A}\frac{30.5}{N_{\rm Avo}} \text{ kJ, and } G_{\rm B} = g_{\rm B}\frac{30.5}{N_{\rm Avo}} \text{ kJ}, \quad (15)$$

respectively, where $N_{\rm Avo} = 6.022 \times 10^{23}\text{mol}^{-1}$ is Avogadro's constant. For multiple bit transmissions, the synthesis cost of type A molecules at the source is

$$E_{\rm S}^{\rm syn} = \sum_{j=1}^{n_{\rm bit}} x_{\rm S}[j] N_{\rm A} G_{\rm A}, \quad (16)$$

where $n_{\rm bit}$ is the total number of bits emitted at the source.

D. Synthesis Cost at the Relay

The chemical reactions are a type of thermodynamic process. The Gibbs free energy is a thermodynamic potential that can be used to calculate the amount of energy required for a reaction to happen in a thermodynamic system [15]. The reactions at the relay require the energy released from hydrolysis of ATP. For one type A molecule converting to m molecules of type B, the standard-state free energy of reaction is given as [16, Ch. 7 Eq. (20)]

$$\text{A} \rightarrow m\text{B}, \quad \Delta G^{\rm AB} = (mG_{\rm B} - G_{\rm A}) \text{ kJ}, \ (m \geq 1) \quad (17)$$

where $\Delta G^{\rm AB}$ is the difference between the free energy of a substance and the free energies of its constituent elements at standard-state conditions, and $G_{\rm A}$ and $G_{\rm B}$ are given in (15).

The expected synthesis cost of type B molecules from type A molecules at the SMIET relay is calculated as

$$E_{\rm R}^{\rm syn} = \sum_{j=1}^{n_{\rm bit}} \hat{x}_{\rm R}[j] N_{\rm A}\Psi_{\rm R}[j] (mG_{\rm B} - G_{\rm A}) \text{ kJ}, (mG_{\rm B} > G_{\rm A}). \quad (18)$$

We note that the synthesis cost at the relay is zero for $mG_{\rm B} \leq G_{\rm A}$, thus (18) provides the maximum synthesis cost at the SMIET

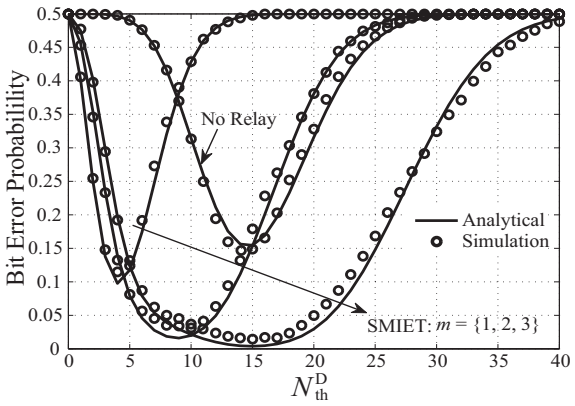

Fig. 1. Bit Error Probability versus the detection threshold at the destination.

relay. As shown in (18), the maximum synthesis cost increases with increasing the expected number of absorbed molecules at the SMIET relay.

E. Synthesis Cost of Molecular Communication System

For the random $n_{\rm bit}$ bits emitted at the source, the expected maximum synthesizing cost of the two-hop molecular communication system can be written as

$$\begin{aligned} E_{\rm tot}^{\rm syn} =& P_1 E_{\rm ET}^{\rm syn}\left(x_{\rm S}[n_{\rm bit}]=1 \middle| x_{\rm S}[1:(n_{\rm bit}-1)]\right) \\ &+ P_0 E_{\rm ET}^{\rm syn}\left(x_{\rm S}[n_{\rm bit}]=0 \middle| x_{\rm S}[1:(n_{\rm bit}-1)]\right), \end{aligned} \quad (19)$$

where

$$\begin{aligned} &E_{\rm ET}^{\rm syn}\left(x_{\rm S}[n_{\rm bit}]=(\cdot) \middle| x_{\rm S}[1:(n_{\rm bit}-1)]\right) \\ &= N_{\rm A}\sum_{j=1}^{n_{\rm bit}}\left[x_{\rm S}[j]G_{\rm A} + \hat{x}_{\rm R}[j]\Psi_{\rm R}[j]\left(mG_{\rm B}-G_{\rm A}\right)\right]. \end{aligned} \quad (20)$$

IV. Numerical Results

In this section, we present the simulation and analytical results. In the figure and the table, we set $N_{\rm A}=100$, $n_{\rm bit}=4$, $d_{\rm R}=d_{\rm D}=R_{\rm R}=R_{\rm D}=4$ μm, $T_{\rm R}=T_{\rm D}=0.5T_b=0.14$ s, $P_0=P_1=0.5$, $N_{\rm th}^{\rm R}=10$, $D_{\rm A}=158.8$ μm^2/s, $D_B=lD_A$, $l\approx m$, $g_{\rm A}=6000$, $g_{\rm B}=4000$, the simulation step is 10^{-5} s, and simulations were repeated 10^3 times[3]. The "Simple Relay" case corresponds to the relay not having SMIET capability, such that it must synthesise type B molecules directly, whereas the "No Relay" case corresponds to no relay in the system[4].

Fig. 1 plots the bit error probabilities at the destination, where the analytical curves are plotted via Eq. (11), and the simulation points are plotted by extending the particle-based simulation algorithm in [7]. Table I presents the synthesis cost corresponding to each case in Fig. 1. We observe that with the SMIET relay, increasing the reaction factor m improves the minimum bit error probability, but increases the synthesis cost, which can be seen from (20). The "No relay" case has the worst minimum bit error probability. The "Simple Relay" and "$m=1$" cases achieve the same bit error probability, but the "$m=1$" case has a much lower synthesis cost, which demonstrates the energy efficiency of the SMIET relay system via molecule type conversion. With the same synthesis cost for the "$m=3$" and "Simple Relay" cases, the "$m=3$" case achieves a much lower minimum bit error probability, which showcases the performance enhancement brought by the SMIET relay.

TABLE I
SYNTHESIS COST OF THE MOLECULAR COMMUNICATION SYSTEM ($\times 10^{-16}$) KJ

Simple Relay	SMIET $m=1$	SMIET $m=2$	SMIET $m=3$	No Relay
1.3121	1.0604	1.1464	1.3121	1.0604

V. Conclusions

In this paper, we proposed and modeled an energy efficient molecular communication system with a SMIET relay. We have examined the bit error probability and synthesis cost of the two-hop molecular communication system with the SMIET relay. Importantly, our results showed that the minimum bit error probability can be greatly improved with low synthesis cost in the SMIET relay system. The extension to a finite reaction rate inside the SMIET relay with counting noise can be considered in future work.

[3]We use $l\approx m$ as a first approximation without considering the specific shapes of A and B. The value of $g_{\rm A}$ corresponds to the typical amount of ATP required to synthesize a protein with $100-200$ amino acids.

[4]To make these comparisons fair, the distance between the source and the center of destination in the "No relay" case is equal to $d_{\rm R}+d_{\rm D}+R_{\rm D}$.

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