






# Energy-Efficient Transmitter Creation in Molecular Communication

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**Abstract.** The availability of molecular resources is of paramount importance in molecular communication (MC), where information is intricately encoded within the properties of molecules. In MC, the acquisition of molecules from the environmental mixture is followed by the essential process of purifying these molecules through controlled transfers between reservoirs, especially for molecular shift keying (MoSK). This paper focuses on a transmitter featuring dual reservoirs designated for the storage of information molecules, with the transference of a specific molecular species from one reservoir to another facilitated by the consumption of free energy. Given the constrained energy resources within the transmitter, we investigate an energy-efficient mechanism for transmitter creation, aimed at optimizing overall transmitter performance. Theoretical analyses are systematically conducted to explore diverse strategies for the movement of molecules between reservoirs. Ultimately, numerical results substantiate the efficacy of the proposed molecular movement strategy in the transmitter creation.

**Keywords:** Molecular resources · Molecular communication · Free energy · Energy-efficient

## 1 Introduction

The rapid advancement of nanotechnology has catalyzed significant breakthroughs in the development of nanomachines, particularly in the applications related to drug delivery and continuous health monitoring [1, 2]. Inspired by natural cell-to-cell communication, molecular communication (MC) has emerged as a promising solution for facilitating communication between nanomachines. In MC, information is encoded within the properties of molecules, such as in the molecule concentration, type, and release time. Subsequently, these encoded molecules are emitted by the transmitter and traverse the medium to reach

the receiver through diffusion-based propagation, flow-assisted propagation, or active transport mechanisms. At the receiver, specialized receptors detect and decode the information carried by the molecules.

In the diffusion-based MC, molecules propagate to the receiver through Brownian motion, a process that does not necessitate the expenditure of free energy. However, the acquisition of molecules—whether through collection from the environment or synthesis by cells—requires the investment of free energy [3,4]. Although the technology of locally synthesizing information molecules by genetically engineered bacteria has achieved significant breakthroughs, the synthesis primarily involves molecules of the same kind. This limitation renders modulation using multiple types of molecules unfeasible, a common practice in MC. Furthermore, the utilization of reservoirs is integral for the transmitter to effectively store these molecules.

Given the inherently constrained energy storage capacity of nanomachines, coupled with limitations in energy harvesting from the surrounding environment [5], the development of an energy-efficient transmitter creation mechanism becomes paramount in MC. In [6], the architecture of the transmitter was thoroughly investigated, with a particular focus on molecular storage and generation. To enhance the efficiency of molecular utilization, the recycling and reutilization of previously released molecules was considered. In the work by Deng et al. [7], the generation of molecules at the relay was investigated, utilizing absorbed molecules through chemical reactions. Lotter et al. [8] explored molecule harvesting in neurons, while Ahmadzadeh et al. [4] delved into mathematical models for molecule harvesting in diffusive MC systems, wherein molecules within harvesting units may be recaptured by the transmitter. Recognizing that the limited storage capacity of the transmitter can impact the performance of the MC system, Rezaei et al. [9] proposed a production unit that exponentially replenishes the transmitter’s storage, ensuring a sufficient quantity of molecules for future transmissions.

In MC systems with relays, the use of multiple types of molecules in information transmission has been explored in past works [10,11]. In [12], the authors employed On-Off keying, utilizing only one type of molecule for modulation. In pursuit of achieving high-rate transmission in MC, [13] utilized DNA as an information carrier, leveraging its high information density and biological compatibility. Furthermore, in [14], a molecular shell mapping scheme was employed to implement probabilistic constellation shaping for MC, enhancing system performance when employing multi-level concentration shift keying.

Our previous work [15] explored the creation of a transmitter through the harvesting of molecules from the environment, and storing them in reservoirs for use by the transmitter. The implementation of Molecule Shift Keying (MoSK) involves the collection of multiple types of molecules. However, the collected molecules form a mixture, rendering MoSK unreliable. Previous research, such as [16], has investigated the energy cost associated with moving molecules between reservoirs. By expending free energy, one type of molecule is transferred from one reservoir to another. Nevertheless, the energy cost increases rapidly with the

number of transferred molecules, resulting in a mixture of molecules within the reservoirs, thus forming an imperfect transmitter.

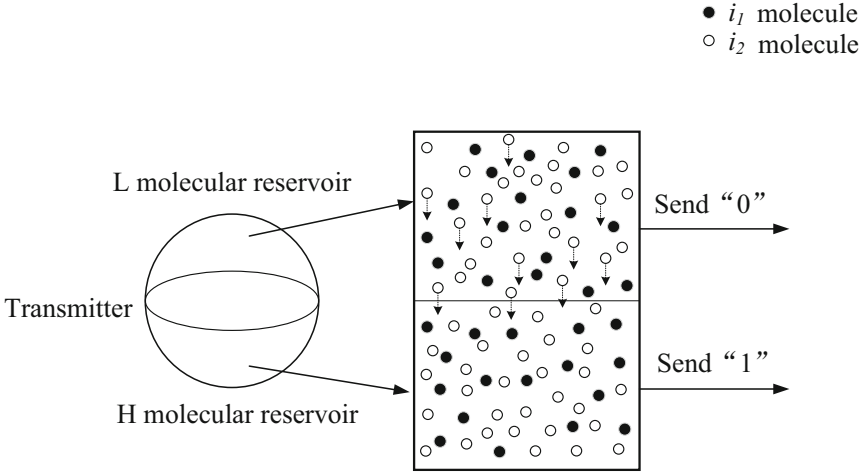
In the study by [17], an imperfect transmitter was considered, where molecules encapsulated within vesicles are released by the transmitter membrane, albeit with a certain probability. Our previous work, as presented in [18], delved into the performance of the imperfect transmitter, created by transferring molecules between reservoirs using free energy. Furthermore, the energy allocation among nanomachines in cooperative MC was investigated. However, both [16, 18] focused on moving a single kind of molecule between reservoirs. Given the constraints of limited energy within nanomachines, achieving energy-efficient transmitter creation is paramount for MC. Therefore, based on the works conducted in [15, 16, 18], which directly assumes the movement of a single type of molecule between reservoirs, this paper investigates the performance of the transmitter under diverse molecule-moving strategies. The primary contribution of this paper lies in the exploration of a highly energy-efficient mechanism for transmitter creation, achieved by examining various strategies for moving molecules between reservoirs.

The subsequent sections of this paper are structured as follows. In Sect. 2, we elucidate the model of the MC system, encompassing the movement of molecules and associated energy consumption. Section 3 undertakes a theoretical analysis of the transmitter, specifically examining the impact of moving various types of molecules. Section 4 is dedicated to the validation of transmitter performance under diverse movement strategies. Ultimately, Sect. 5 encapsulates the conclusion of this paper.

## 2 System Model

The system model considered in this paper consists of two molecular reservoirs,  $L$  and  $H$ , at the transmitter. The transmitter collects two types of information molecules from the environment,  $i_1$  and  $i_2$ , which do not react with each other. The collected molecules are uniformly distributed in the container of the transmitter due to diffusion, so the distribution of the two types of molecules in the molecular reservoirs is completely the same in the initial state. Therefore, the total number and concentration of molecules in the two molecular reservoirs are the same initially. Subsequently, by consuming energy to move a certain type of molecule, the distribution of molecule concentrations in the  $L$  and  $H$  molecular reservoirs is changed, forming an imperfect transmitter.

Figure 1 shows the process of forming an imperfect transmitter, where the larger initial concentration of the  $i_2$  molecules in the  $L$  molecular reservoir is moved by consuming energy to create a concentration difference between the two molecular reservoirs, resulting in an imperfect transmitter. The molecules released from the  $L$  molecular reservoir represent the transmission bit 0, while the molecules released from the  $H$  molecular reservoir represent the transmission bit 1.



**Fig. 1.** The process of consuming energy to move  $i_2$  molecules to form an imperfect transmitter.

Assuming that in the initial state, the concentrations of  $i_2$  molecules in the  $L$  and  $H$  reservoirs are both  $c_2$ , where  $c_2$  is equal to the ratio of the total number of  $i_2$  molecules in each reservoir to the total number of molecules in that reservoir, the concentration of  $i_1$  molecules is  $1 - c_2$ . The total number of molecules in the transmitter is  $n_i = n_{i,L} + n_{i,H}$ , and since the number of molecules in the  $L$  and  $H$  molecular reservoirs are equal in the initial state, it is denoted as  $n_{i,L} = n_{i,H} = \frac{1}{2}n_i$ .

Considering the input energy is constant and the initial concentrations of the two types of molecules are different, the number of molecules that can be moved by moving different molecules is different. Therefore, we first analyze the relationship between the input energy and the number of molecules that can be moved.

Assuming  $m_2$   $i_2$  molecules are moved, where  $m_2$  is the number of moved  $i_2$  molecules, and  $m_2 \ll \frac{n_i}{2}$ , therefore, the number of  $i_2$  molecules that can be moved under given energy can be expressed as [18]

$$m_2 = \sqrt{\frac{c_2 n_i}{2KT}} E. \tag{1}$$

Similarly, assuming  $m_1$   $i_1$  molecules are moved, where  $m_1$  is the number of moved  $i_1$  molecules,  $m_1 \ll \frac{n_i}{2}$ , and  $c_1 = 1 - c_2$ , therefore, the number of moved  $i_1$  molecules under a given energy can be expressed as

$$m_1 = \sqrt{\frac{(1 - c_2) n_i}{2KT}} E. \tag{2}$$

From Eqs. (1) and (2), it can be seen that the number of molecules that can be moved,  $m$ , is related to the input energy  $E$  and the initial concentration of the

molecule being moved  $c$ . Under the same given energy, the number of molecules that can be moved is determined by the initial concentration of the molecule, with a larger initial concentration resulting in a larger number of molecules that can be moved. Moreover, under the same conditions,  $m_1$  and  $m_2$  can be considered as a univariate function of the molecule  $i_2$  initial concentration  $c_2$ . It can be observed that  $m_1(1 - c_2) = m_2(c_2)$ , indicating that  $m_1$  and  $m_2$  are symmetric with respect to  $c_2 = 0.5$ .

Therefore, the considered transmitter model consists of two molecular reservoirs,  $L$  and  $H$ , which store both mixture molecules  $i_1$  and  $i_2$ . In the initial state, the concentrations of all types of molecules in both  $L$  and  $H$  reservoirs are the same. By consuming energy, we can move a certain number of a specific type of molecule, causing a difference in the concentration distribution of molecules in the two reservoirs. This allows the transmitter to emit molecules with different concentration distributions, encoding bit 1 and bit 0 on the molecules in the  $H$  and  $L$  reservoirs, respectively, resulting in an imperfect transmitter. However, as the energy is limited, and the energy cost increases rapidly with the number of moved molecules, therefore, in the next section, we explore the strategies for constructing imperfect transmitters with lower energy consumption and lower error rates.

### 3 Performance Analysis of Imperfect Transmitters When Moving Different Molecules

The performance of the imperfect transmitter under consideration is influenced by both the energy cost and the strategies employed for moving molecules. Improper handling of these factors can lead to elevated error rates and inefficient utilization of energy resources. Consequently, it holds great significance to investigate the interplay between transmitter performance and molecule movement strategies. Such a study is crucial for designing a highly efficient transmitter within the MC system.

In the initial state, the concentrations of  $i_2$  molecules in both  $L$  and  $H$  reservoirs are  $c_2$ , and the concentration of  $i_1$  molecules is  $1 - c_2$ . The ratio of the initial concentrations of  $i_1$  and  $i_2$  molecules in  $L$  and  $H$  reservoirs can be expressed as

$$c_{i_1,L}/c_{i_2,L} = c_{i_1,H}/c_{i_2,H} = \frac{1}{c_2} - 1. \quad (3)$$

Then, utilizing the concentration variances resulting from the movement of different molecules, a decision rule based on the ratio of concentrations of distinct molecules at the receiver is introduced. The statistical characteristics of the received molecules are analyzed to explore the relationship between transmitter performance, energy cost, and the initial state of molecules in the reservoirs, aiming to characterize the system's efficiency. Through a comparison of the transmitter's performance under different movement strategies, a method for moving molecules is identified, leading to the creation of a more efficient transmitter with limited energy input.

### 3.1 Moving $i_2$ Molecules from $L$ to $H$ Reservoir

When  $m_2$   $i_2$  molecules are moved from the  $L$  reservoir to the  $H$  reservoir, considering that  $m_2 \ll \{n_{i,L}, n_{i,H}\}$ , the concentrations of molecules in the  $L$  and  $H$  reservoirs can be approximated as

$$\begin{cases} c_{i_2,L} = \frac{n_{i,L}c_2 - m_2}{n_{i,L}} = c_2 - \frac{m_2}{n_{i,L}}, \\ c_{i_2,H} = \frac{n_{i,H}c_2 + m_2}{n_{i,H}} = c_2 + \frac{m_2}{n_{i,H}}. \end{cases} \quad (4)$$

After moving  $m_2$   $i_2$  molecules from the  $L$  reservoir to the  $H$  reservoir, the ratio of  $i_1$  and  $i_2$  molecules in the  $L$  reservoir increases, making  $c_{i_1,L}/c_{i_2,L} \geq \frac{1}{c_2} - 1$ , while the ratio in the  $H$  reservoir decreases,  $c_{i_1,H}/c_{i_2,H} < \frac{1}{c_2} - 1$ . Therefore, the decision criterion for the information carried by the released molecules by the transmitter can be expressed as

$$b_{rx,i} = \begin{cases} 0, c_{i_1,L}/c_{i_2,L} \geq \frac{1}{c_2} - 1, \\ 1, c_{i_1,H}/c_{i_2,H} < \frac{1}{c_2} - 1. \end{cases} \quad (5)$$

Thus, if the ratio of the two molecular concentrations detected by the receiver satisfies  $c_{i_1,L}/c_{i_2,L} \geq \frac{1}{c_2} - 1$ , it is determined that bit 0 has been received. Conversely, if the ratio of the two molecular concentrations satisfies  $c_{i_1,H}/c_{i_2,H} < \frac{1}{c_2} - 1$ , it is determined that bit 1 has been received.

Assuming  $M$  is the number of molecules emitted by the transmitter, to correctly transmit bit 0, it should satisfy  $c_{i_1,L}/c_{i_2,L} \geq \frac{1}{c_2} - 1$ . It can be derived that the minimum number of  $i_1$  molecules emitted from the  $L$  reservoir should be  $\lfloor M(1 - c_2) \rfloor + 1$ , so the probability of correctly transmitting bit 0 can be expressed as

$$P_{i_2}(Y = 0 | X = 0) = \frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,L}(1-c_{i_2,L})}^i C_{n_{i,L}c_{i_2,L}}^{M-i}}{C_{n_{i,L}}^M}. \quad (6)$$

Similarly, for sending bit 1, the probability of correctly transmitting the molecules at the receiver can be expressed as

$$P_{i_2}(Y = 1 | X = 1) = \frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,H}c_{i_2,H}}^i C_{n_{i,H}(1-c_{i_2,H})}^{M-i}}{C_{n_{i,H}}^M}. \quad (7)$$

Assuming the probability of transmitting bit 0 or 1 is both 0.5, the error rate used to characterize the transmitter performance when moving molecules  $i_2$  is

$$\begin{aligned}
 P_{e,i_2} &= P(X=0) \cdot P(Y=1|X=0) + P(X=1) \cdot P(Y=0|X=1) \\
 &= \frac{1}{2} \left[ (1 - P_{i_2}(Y=0|X=0)) + (1 - P_{i_2}(Y=1|X=1)) \right] \\
 &= \frac{1}{2} \left( 2 - \frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,L}}^i (1-c_{i_2,L})^{M-i} C_{n_{i,L}}^{M-i} c_{i_2,L}^i}{C_{n_{i,L}}^M} - \frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,H}}^i c_{i_2,H}^{M-i} C_{n_{i,H}}^{M-i} (1-c_{i_2,H})^i}{C_{n_{i,H}}^M} \right), \tag{8}
 \end{aligned}$$

where  $\frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,L}}^i (1-c_{i_2,L})^{M-i} C_{n_{i,L}}^{M-i} c_{i_2,L}^i}{C_{n_{i,L}}^M}$  follows a hypergeometric distribution, and as  $n_{i,L}$  is large, this distribution can be approximated by a binomial distribution  $X_{i_2,0}(i) \sim B(i, 1 - c_{i_2,L})$ . Considering that  $M$  is also large, the binomial distribution can be further approximated by a normal distribution  $X_{i_2,0}(i) \sim N(i, 1 - c_{i_2,L})$ , where

$$\begin{aligned}
 \mu_0 &= M(1 - c_{i_2,L}), \\
 \sigma_0^2 &= Mc_{i_2,L}(1 - c_{i_2,L}). \tag{9}
 \end{aligned}$$

Therefore, the probability of sending bit 0 and correctly judging it can be approximated as

$$P_{i_2}(Y=0|X=0) = \Phi\left(\frac{M - \mu_0}{\sigma_0}\right) - \Phi\left(\frac{\lfloor M(1 - c_2) \rfloor + 1 - \mu_0}{\sigma_0}\right), \tag{10}$$

where  $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-\frac{t^2}{2}} dt$ , the cumulative distribution function of the standard normal distribution.

In molecular communication, assuming  $M(1 - c_2)$  is large, we can approximate  $\lfloor M(1 - c_2) \rfloor + 1 - \mu_0$  as  $M(1 - c_2) - \mu_0$ , so Eq. (10) can be written as

$$P_{i_2}(Y=0|X=0) = \Phi\left(\frac{M - \mu_0}{\sigma_0}\right) - \Phi\left(\frac{M(1 - c_2) - \mu_0}{\sigma_0}\right). \tag{11}$$

Similarly, by considering the large values of  $n_{i,H}$  and  $M$ , the hypergeometric distribution  $\frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,H}}^i c_{i_2,H}^{M-i} C_{n_{i,H}}^{M-i} (1-c_{i_2,H})^i}{C_{n_{i,H}}^M}$  can be approximated as binomial distribution, and further approximated as normal distribution  $X_{i_2,1}(i) \sim N(i, c_{i_2,H})$ , where

$$\begin{aligned}
 \mu_1 &= Mc_{i_2,H}, \\
 \sigma_1^2 &= Mc_{i_2,H}(1 - c_{i_2,H}). \tag{12}
 \end{aligned}$$

Therefore, the probability of sending bit 1 and correctly judging it can be approximated as

$$P_{i_2}(Y=1|X=1) = \Phi\left(\frac{M - \mu_1}{\sigma_1}\right) - \Phi\left(\frac{\lfloor Mc_2 \rfloor + 1 - \mu_1}{\sigma_1}\right). \tag{13}$$

Similarly, in molecular communication, assuming  $Mc_2$  is large, we can approximate  $\lfloor Mc_2 \rfloor + 1 - \mu_1$  as  $Mc_2 - \mu_1$ , so Eq. (13) can be written as

$$P_{i_2}(Y = 1 | X = 1) = \Phi\left(\frac{M - \mu_1}{\sigma_1}\right) - \Phi\left(\frac{Mc_2 - \mu_1}{\sigma_1}\right). \quad (14)$$

Therefore, when  $i_2$  molecules are moved, the error rate of transmitting information in a time slot by the transmitter can be approximated as

$$\begin{aligned} P_{e,i_2} &= \frac{1}{2} \left[ 2 - \Phi\left(\frac{M - \mu_0}{\sigma_0}\right) + \Phi\left(\frac{M(1 - c_2) - \mu_0}{\sigma_0}\right) - \Phi\left(\frac{M - \mu_1}{\sigma_1}\right) + \Phi\left(\frac{Mc_2 - \mu_1}{\sigma_1}\right) \right] \\ &= \frac{1}{2} \left[ 2 - \Phi\left(\frac{Mc_{i_2,L}}{\sqrt{Mc_{i_2,L}(1 - c_{i_2,L})}}\right) + \Phi\left(\frac{M(c_{i_2,L} - c_2)}{\sqrt{Mc_{i_2,L}(1 - c_{i_2,L})}}\right) \right. \\ &\quad \left. - \Phi\left(\frac{M(1 - c_{i_2,H})}{\sqrt{Mc_{i_2,H}(1 - c_{i_2,H})}}\right) + \Phi\left(\frac{M(c_2 - c_{i_2,H})}{\sqrt{Mc_{i_2,H}(1 - c_{i_2,H})}}\right) \right]. \end{aligned} \quad (15)$$

Substituting Eq. (4), the final expression for the error rate when moving  $i_2$  molecules can be obtained as

$$\begin{aligned} P_{e,i_2} &= \frac{1}{2} \left[ 2 - \Phi\left(\frac{M(c_2 - \frac{m_2}{n_{i,L}})}{\sqrt{M(c_2 - \frac{m_2}{n_{i,L}})(1 - c_2 + \frac{m_2}{n_{i,L}})}}\right) + \Phi\left(\frac{-M \frac{m_2}{n_{i,L}}}{\sqrt{M(c_2 - \frac{m_2}{n_{i,L}})(1 - c_2 + \frac{m_2}{n_{i,L}})}}\right) \right. \\ &\quad \left. - \Phi\left(\frac{M(1 - c_2 - \frac{m_2}{n_{i,H}})}{\sqrt{M(c_2 + \frac{m_2}{n_{i,H}})(1 - c_2 - \frac{m_2}{n_{i,H}})}}\right) + \Phi\left(\frac{-M \frac{m_2}{n_{i,H}}}{\sqrt{M(c_2 + \frac{m_2}{n_{i,H}})(1 - c_2 - \frac{m_2}{n_{i,H}})}}\right) \right], \end{aligned} \quad (16)$$

where  $M$  is the number of molecules emitted by the transmitter,  $c_2$  is the initial concentration of  $i_2$  molecules, and  $m_2 = \sqrt{\frac{c_2 n_i}{2KT} E}$ .

### 3.2 Moving $i_1$ Molecules from $L$ to $H$ Reservoir

When  $m_1$   $i_1$  molecules are moved from the  $L$  reservoir to the  $H$  reservoir, considering that  $m_1 \ll n_{i,L}, n_{i,H}$ , the concentrations of  $i_2$  molecules in the  $L$  and  $H$  reservoirs can be approximated as follows

$$\begin{cases} c_{i_2,L} = 1 - c_{i_1,L} = 1 - \frac{n_{i,L}(1 - c_2) - m_1}{n_{i,L}} = c_2 + \frac{m_1}{n_{i,L}}, \\ c_{i_2,H} = 1 - c_{i_1,H} = 1 - \frac{n_{i,H}(1 - c_2) + m_1}{n_{i,H}} = c_2 - \frac{m_1}{n_{i,H}}. \end{cases} \quad (17)$$

After moving  $m_1$   $i_1$  molecules from the  $L$  reservoir to the  $H$  reservoir, the ratio of  $i_1$  and  $i_2$  molecules in the  $L$  reservoir decreases, that is  $c_{i_1,L}/c_{i_2,L} \leq \frac{1}{c_2} - 1$ , while the ratio in the  $H$  reservoir increases, that is  $c_{i_1,H}/c_{i_2,H} > \frac{1}{c_2} - 1$ .

Therefore, the decision criterion for the information carried by the molecular stream emitted by the transmitter can be expressed as

$$b_{rx,i} = \begin{cases} 0, & c_{i_1,L}/c_{i_2,L} \leq \frac{1}{c_2} - 1, \\ 1, & c_{i_1,H}/c_{i_2,H} > \frac{1}{c_2} - 1. \end{cases} \quad (18)$$

Thus, if the ratio of two molecular concentrations detected by the receiver satisfies  $c_{i_1,L}/c_{i_2,L} \leq \frac{1}{c_2} - 1$ , then, bit 0 has been received, otherwise, bit 1 has been received.

Assuming  $M$  is the number of molecules emitted by the transmitter, to correctly receive bit 0, it should satisfy  $c_{i_1,L}/c_{i_2,L} \leq \frac{1}{c_2} - 1$ . It can be derived that the minimum number of  $i_2$  molecules emitted from the  $L$  reservoir should be  $\lfloor Mc_2 \rfloor + 1$ , so the probability of correctly transmitting bit 0 can be expressed as

$$P_{i_1}(Y = 0 | X = 0) = \frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,L}c_{i_2,L}}^i C_{n_{i,L}(1-c_{i_2,L})}^{M-i}}{C_{n_{i,L}}^M}. \quad (19)$$

Similarly, for sending bit 1, the probability of correctly receiving it at the receiver is

$$P_{i_1}(Y = 1 | X = 1) = \frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,H}(1-c_{i_2,H})}^i C_{n_{i,H}c_{i_2,H}}^{M-i}}{C_{n_{i,H}}^M}. \quad (20)$$

Assuming the probability of transmitting bit 0 or 1 is both 0.5, the error rate used to characterize the transmitter performance when moving  $i_1$  molecules is

$$\begin{aligned} P_{e,i_1} &= P(X = 0) \cdot P(Y = 1 | X = 0) + P(X = 1) \cdot P(Y = 0 | X = 1) \\ &= \frac{1}{2} \left[ (1 - P_{i_1}(Y = 0 | X = 0)) + (1 - P_{i_1}(Y = 1 | X = 1)) \right] \\ &= \frac{1}{2} \left( 2 - \frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,L}c_{i_2,L}}^i C_{n_{i,L}(1-c_{i_2,L})}^{M-i}}{C_{n_{i,L}}^M} - \frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,H}(1-c_{i_2,H})}^i C_{n_{i,H}c_{i_2,H}}^{M-i}}{C_{n_{i,H}}^M} \right), \end{aligned} \quad (21)$$

where  $\frac{\sum_{i=\lfloor Mc_2 \rfloor + 1}^M C_{n_{i,L}c_{i_2,L}}^i C_{n_{i,L}(1-c_{i_2,L})}^{M-i}}{C_{n_{i,L}}^M}$  and  $\frac{\sum_{i=\lfloor M(1-c_2) \rfloor + 1}^M C_{n_{i,H}(1-c_{i_2,H})}^i C_{n_{i,H}c_{i_2,H}}^{M-i}}{C_{n_{i,H}}^M}$  are hypergeometric distributions of random variables  $i$ . The simplification and analysis process after this part is similar to that of the first moving method. Finally,

when  $i_1$  molecules are moved, the error rate of transmitting information in a time slot by the transmitter can be approximated as

$$\begin{aligned}
P_{e,i_1} &= \frac{1}{2} \left[ 2 - \Phi\left(\frac{M - \mu_0}{\sigma_0}\right) + \Phi\left(\frac{Mc_2 - \mu_0}{\sigma_0}\right) - \Phi\left(\frac{M - \mu_1}{\sigma_1}\right) + \Phi\left(\frac{M(1 - c_2) - \mu_1}{\sigma_1}\right) \right] \\
&= \frac{1}{2} \left[ 2 - \Phi\left(\frac{M(1 - c_{i_2,L})}{\sqrt{Mc_{i_2,L}(1 - c_{i_2,L})}}\right) + \Phi\left(\frac{M(c_2 - c_{i_2,L})}{\sqrt{Mc_{i_2,L}(1 - c_{i_2,L})}}\right) \right. \\
&\quad \left. - \Phi\left(\frac{Mc_{i_2,H}}{\sqrt{Mc_{i_2,H}(1 - c_{i_2,H})}}\right) + \Phi\left(\frac{M(c_{i_2,H} - c_2)}{\sqrt{Mc_{i_2,H}(1 - c_{i_2,H})}}\right) \right].
\end{aligned} \tag{22}$$

Substituting Eq. (17), the final expression for the error rate when moving  $i_1$  molecules can be obtained as

$$\begin{aligned}
P_{e,i_1} &= \frac{1}{2} \left[ 2 - \Phi\left(\frac{M(1 - c_2 - \frac{m_1}{n_{i,L}})}{\sqrt{M(c_2 + \frac{m_1}{n_{i,L}})(1 - c_2 - \frac{m_1}{n_{i,L}})}}\right) + \Phi\left(\frac{-M\frac{m_1}{n_{i,L}}}{\sqrt{M(c_2 + \frac{m_1}{n_{i,L}})(1 - c_2 - \frac{m_1}{n_{i,L}})}}\right) \right. \\
&\quad \left. - \Phi\left(\frac{M(c_2 - \frac{m_1}{n_{i,H}})}{\sqrt{M(c_2 - \frac{m_1}{n_{i,H}})(1 - c_2 + \frac{m_1}{n_{i,H}})}}\right) + \Phi\left(\frac{-M\frac{m_1}{n_{i,H}}}{\sqrt{M(c_2 - \frac{m_1}{n_{i,H}})(1 - c_2 + \frac{m_1}{n_{i,H}})}}\right) \right],
\end{aligned} \tag{23}$$

where  $M$  is the total number of molecules emitted by the transmitter,  $c_2$  is the initial concentration of  $i_2$  molecules, and  $m_1 = \sqrt{\frac{(1-c_2)n_i}{2KT} E}$ .

From Eq. (16) and Eq. (23), it can be concluded that under the same conditions,  $P_{e,i_1}$  and  $P_{e,i_2}$  can be considered as a univariate function of  $c_2$ , and it can be observed that  $P_{e,i_1}(1 - c_2) = P_{e,i_2}c_2$ , indicating that  $P_{e,i_1}$  and  $P_{e,i_2}$  are symmetric with respect to  $c_2 = 0.5$ . This indicates that under the same conditions, for the error rates  $P_{e,i_2}$  generated by moving  $i_2$  molecules and  $P_{e,i_1}$  generated by moving  $i_1$  molecules at the transmitter, the changes with respect to  $c_2$  are symmetric with respect to  $c_2 = 0.5$ . Furthermore, it can be inferred that under the same energy cost to create an imperfect transmitter, the higher the concentration of the moved molecules, the lower the error rate of the transmitter.

In this paper, we consider that all information molecules are collected only once before transmission. Given that the total number of collected molecules in the reservoirs significantly exceeds the number of emitted molecules per bit, the molecular resources are sufficient for the communication process.

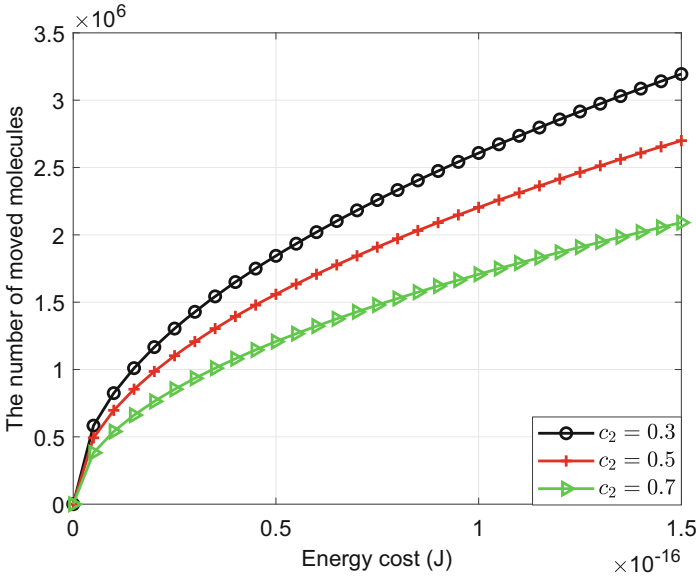
## 4 Numerical and Simulation Results

In this section, based on the above analysis, we delve into the relationship between energy consumption and the number of moved molecules, along with the transmitter's performance under different initial concentrations of molecules. Additionally, we explore the relationship between the initial concentration of the molecule and the Bit Error Rate (BER) when different molecules are moved with

a fixed input energy. The simulation parameters used include the Boltzmann constant  $K = 1.3807 \cdot 10^{-23} \text{ J/K}$ , absolute temperature  $T = 298.15 \text{ K}$ , the number of molecules emitted by the transmitter  $M = 5000$ , total number of molecules in the  $L$  reservoir and  $H$  reservoir  $n_{i,L} = n_{i,H} = 4 \cdot 10^8$ , and total number of molecules at the transmitter  $n_i = n_{i,L} + n_{i,H} = 8 \cdot 10^8$ .

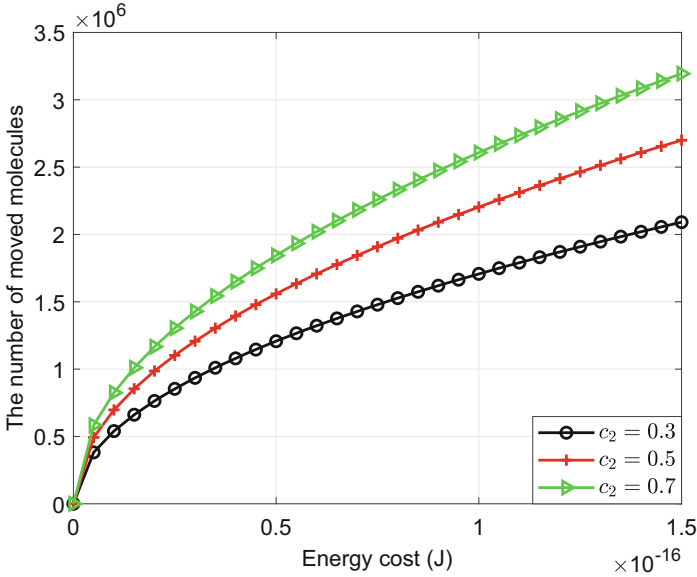
Figures 2 and 3 depict the relationship between energy consumption and the number of moved molecules for  $i_1$  and  $i_2$  under different initial concentrations. We choose the initial concentration of molecule  $i_2$  as  $c_2 = 0.3$ ,  $c_2 = 0.5$ , and  $c_2 = 0.7$ . Horizontally, the number of moved molecules increases with the rise in input energy for various initial concentrations. Generally, a square root relationship exists between the number of movable molecules and input energy, with the number of moved molecules increasing alongside the initial concentration of moved molecules.

Figure 2 reveals that when moving molecule  $i_1$ , lower initial concentrations of molecule  $i_2$  (higher initial concentration of molecule  $i_1$ ) demand less energy to move the same number of molecules. Meanwhile, Fig. 3 demonstrates that when moving molecule  $i_2$ , higher initial concentrations of molecule  $i_2$  require less energy to move the same number of molecules.



**Fig. 2.** The number of moved molecules  $i_1$  versus the energy cost  $E$  under the different initial concentrations of  $i_2$  molecules  $c_2$  in the reservoirs.

Figures 4 and 5 illustrate the relationship between energy consumption and the BER of the transmitter for different molecules under varying initial concentrations. We select the initial concentration of molecule  $i_2$  as  $c_2 = 0.3$ ,  $c_2 = 0.5$ ,



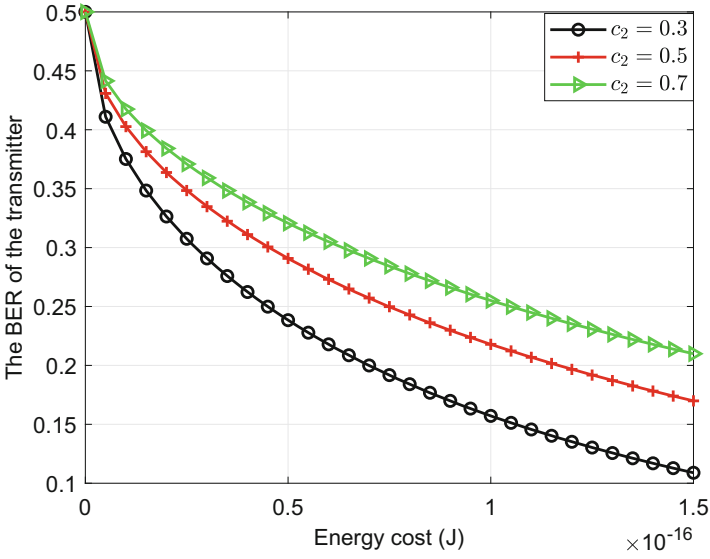
**Fig. 3.** The number of moved molecules  $i_2$  versus the energy cost  $E$  under the different initial concentrations of  $i_2$  molecules  $c_2$  in the reservoirs.

and  $c_2 = 0.7$ . Horizontally, the BER decreases with increased energy consumption under different initial concentrations. This is attributed to the ability of higher energy to move more molecules, altering the concentration distribution in the emitted molecular flow at the transmitter. Consequently, the probabilities  $P(Y = 0 | X = 0)$  and  $P(Y = 1 | X = 1)$  of correctly transmitted information rise, resulting in a lower BER.

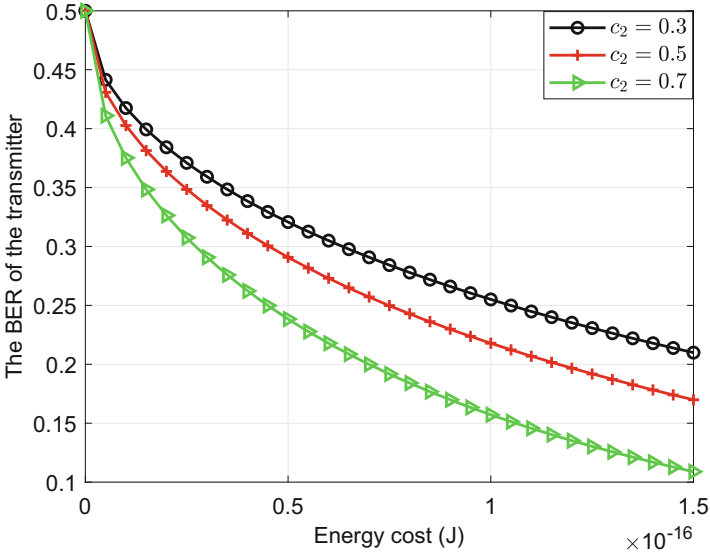
Figure 4 indicates that when moving molecule  $i_1$ , achieving the same BER requires less energy with a lower initial concentration of molecule  $i_2$  (higher initial concentration of molecule  $i_1$ ). Similarly, Fig. 5 demonstrates that when moving molecule  $i_2$ , less energy is needed to achieve the same BER with a higher initial concentration of molecule  $i_2$ .

Vertically, with the same input energy, a higher initial concentration of moved molecules corresponds to a lower BER. Figure 4 reveals that when moving molecule  $i_1$ , lower initial concentrations of molecule  $i_2$  and higher initial concentrations of molecule  $i_1$  lead to a lower BER. Similarly, Fig. 5 shows that when moving molecule  $i_2$ , higher initial concentrations of molecule  $i_2$  result in a lower BER.

Figure 6 illustrates the relationship between the initial concentration of molecule  $i_2$  and the system BER under different types of molecule movements, with a fixed input energy of  $E = 0.875 \cdot 10^{-16} J$ . As shown in Fig. 6, an increase in the initial concentration of molecule  $i_2$  leads to a continuous increase in the BER when molecule  $i_1$  is moved, whereas the BER continuously decreases when molecule  $i_2$  is moved. This behavior is attributed to the



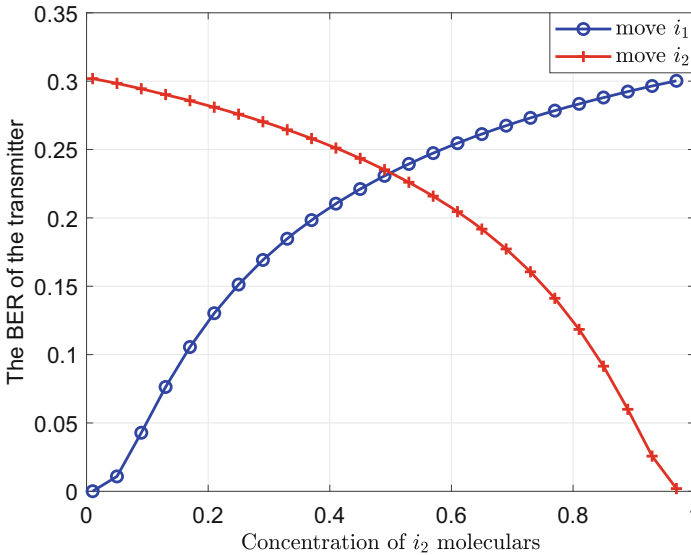
**Fig. 4.** The BER of the transmitter versus the energy cost  $E$  moving  $i_1$  molecules under the different initial concentrations of  $i_2$  molecules  $c_2$  in the reservoirs, holding  $M$  constant.



**Fig. 5.** The BER of the transmitter versus the energy cost  $E$  moving  $i_2$  molecules under the different initial concentrations of  $i_2$  molecules  $c_2$  in the reservoirs, holding  $M$  constant.

larger initial concentration of  $i_2$  molecules, which results in lower energy consumption for moving  $i_2$  molecules and higher energy consumption for moving  $i_1$  molecules. Moreover, Fig. 6 also reveals that the BER for moving the two types of molecules is symmetric around  $c_2 = 0.5$ , which aligns with the derived result of  $P_{e,i_1}(1 - c_2) = P_{e,i_2}(c_2)$ . Therefore, in constructing an imperfect transmitter with energy consumption considerations, moving molecules with higher initial concentrations results in a lower BER and enhances the transmitter's performance.

It can be concluded that, if the initial concentration of  $i_2$  molecules is relatively high, the movement of  $i_2$  molecules results in an imperfect transmitter with a lower BER and enhanced performance. Similarly, if the initial concentration of  $i_1$  molecules is relatively high, the movement of  $i_1$  molecules leads to an imperfect transmitter with a lower BER and improved system performance.



**Fig. 6.** The BER of the transmitter versus the initial concentrations of  $i_2$  molecules  $c_2$  under moving different molecules, holding energy cost  $E$  constant.

## 5 Conclusion

In this paper, our primary focus was on the creation of an imperfect transmitter through the utilization of free energy to facilitate the movement of molecules between the reservoirs. To enhance the energy efficiency of the imperfect transmitter, we analyzed various movement strategies for molecules between the reservoirs. Theoretical and simulation results consistently demonstrated that higher concentrations of the moved molecules corresponded to the BER of the transmitter. This relationship held true as more molecules were moved among the

reservoirs, resulting in a larger gap in the concentration ratio of the two types of molecules between the reservoirs. As a result, in practical applications where the construction of an imperfect transmitter is necessary, superior performance and lower BER can be achieved by expending free energy to move molecules with initially higher concentrations. This finding underscores the significance of thoughtful energy consumption in optimizing the performance of imperfect transmitters.

## References

1. Farsad, N., Yilmaz, H.B., Eckford, A., Chae, C.-B., Guo, W.: A comprehensive survey of recent advancements in molecular communication. *IEEE Commun. Surv. Tutorials* **18**(3), 1887–1919 (2016)
2. Sun, Y., Zhang, R., Chen, Y.: A molecular communication detection method for the deformability of erythrocyte membrane in blood vessels. *IEEE Trans. Nanobiosci.* **20**(4), 387–395 (2021)
3. Kuran, M.Ş, Yilmaz, H.B., Tugcu, T., Özerman, B.: Energy model for communication via diffusion in nanonetworks. *Nano Commun. Netw.* **1**(2), 86–95 (2010)
4. Ahmadzadeh, A., Jamali, V., Schober, R.: Molecule harvesting transmitter model for molecular communication systems. *IEEE Open J. Commun. Soc.* **3**, 391–410 (2022)
5. Wang, J.: *Nanomachines: fundamentals and applications*. John Wiley & Sons (2013)
6. Kuscü, M., Dinc, E., Bilgin, B.A., Ramezani, H., Akan, O.B.: Transmitter and receiver architectures for molecular communications: a survey on physical design with modulation, coding, and detection techniques. *Proc. IEEE* **107**(7), 1302–1341 (2019)
7. Deng, Y., Guo, W., Noel, A., Nallanathan, A., Elkashlan, M.: Enabling energy efficient molecular communication via molecule energy transfer. *IEEE Commun. Lett.* **21**(2), 254–257 (2016)
8. Lotter, S., Ahmadzadeh, A., Schober, R.: Synaptic channel modeling for DMC: neurotransmitter uptake and spillover in the tripartite synapse. *IEEE Trans. Commun.* **69**(3), 1462–1479 (2020)
9. Rezaei, M., Rudsari, H.K., Javan, M., Mokari, N., Jorswieck, E.A., Orooji, M.: Molecular communication transmitter design in limited-capacity storage regime. *IEEE Trans. Nanobiosci.* **22**(2), 212–222 (2022)
10. Cheng, Z., Yan, J., Tu, Y., Chi, K., Xia, M.: Mobile two-way molecular communication via diffusion using amplify-and-forward and analog network coding. *IEEE Trans. Nanobiosci.* **21**(2), 273–285 (2021)
11. Cheng, Z., Yan, J., Sun, J., Tu, Y., Chi, K.: Joint optimizations of relays locations and decision threshold for multi-hop diffusive mobile molecular communication with drift. *IEEE Trans. Nanobiosci.* **21**(3), 454–465 (2022)
12. Jing, D., Li, Y., Eckford, A.W.: An extended kalman filter for distance estimation and power control in mobile molecular communication. *IEEE Trans. Commun.* **70**(7), 4373–4385 (2022)
13. Wang, Q., Sun, Y., Cheng, W., Chen, Y., Yang, K.: Novel interleaved code for high-throughput parallel DNA-based molecular communications. *IEEE Communications Letters* (2023)

14. Tang, Y., Ji, F., Wen, M., Wang, Q., Chae, C.-B., Yang, L.-L.: Probabilistic constellation shaping for molecular communications. *IEEE Trans. Commun.* **71**(9), 5124–5136 (2023)
15. Jing, D., Lin, L., Eckford, A.W.: Thermodynamic energy cost and bit error rate of imperfect transmitters in molecular communication. In: *GLOBECOM 2023 - 2023 IEEE Global Communications Conference*, pp. 552–557 (2023)
16. Eckford, A.W., Kuznets-Speck, B., Hinczewski, M., Thomas, P.J.: Thermodynamic properties of molecular communication. In: *IEEE International Symposium on Information Theory (ISIT)*. IEEE vol. 2018, pp. 2545–2549 (2018)
17. Huang, X., Fang, Y., Noel, A., Yang, N.: Membrane fusion-based transmitter design for static and diffusive mobile molecular communication systems. *IEEE Trans. Commun.* **70**(1), 132–148 (2021)
18. Jing, D., Lin, L., Eckford, A.W.: Energy allocation for multi-user cooperative molecular communication systems in the internet of bio-Nano things. *IEEE Internet Things J.* (2024)