






ISI Mitigation with Molecular Degradation in Molecular Communication

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Abstract. Inter-symbol interference (ISI) decreases the performance of diffusion based molecular communication (MC) significantly. Especially, considering the molecular degradation during the propagation, the ISI mitigation becomes more tricky as the received molecules vary greatly. To tackle this problem, in this paper, we propose an optimal detection method based on maximum likelihood detection by minimizing the error probability. To characterize the proposed detection method, the optimal detection threshold and bit error rate (BER) is derived. Simulation results verified the effectiveness of the proposed ISI mitigation method in the considered MC system with molecular degradation.

Keywords: Inter-symbol interference · Molecular degradation · Molecular communication · Maximum likelihood

1 Introduction

Inspired by the nature communication between biological cells, a new communication paradigm named molecular communication (MC) is proposed which enables the communication between the nanomachines [1, 2]. In the MC, biochemical molecules are employed as the information carriers to transmit the information. MC has broad various promising applications such as in-body health monitoring, drug delivery, etc. [3]. Especially, during the outbreak of COVID-19, MC can also be employed to model the propagation of the virus [4–6].

In MC, the information can be encoded in the molecular concentrations, molecular types, and the release time of molecules. Then the encoded molecules are released into the medium and propagate to the receiver by diffusion, active transport, and others. At the receiver, the nanomachine senses the received molecules and decodes the information.

Diffusion-based molecular communication (DBMC) attracts more attention to its energy efficiency. In DBMC, the released molecules diffuse to the receiver by

Brownian motion making the molecules follow different trajectories and making the channel memory. Therefore, the DBMC suffers from intersymbol interference (ISI) due to the previously released molecules arriving at the receiver in the subsequent time slots.

The ISI decreases the performance of the DBMC greatly. Therefore, various methods have been proposed to mitigate the ISI. In [2], a chemical reaction based method is proposed where acids, bases, and the concentration of hydrogen ions are employed to transmit the information. In [7], a pre-equalization scheme where the difference between the number of received two types of molecules as the actual signal is proposed to mitigate the ISI. In [8], to mitigate the ISI, the increase of the received molecular concentration rather than the absolute concentration is considered. By employing the K-means clustering algorithm, in [9], the detection thresholds can be reformulated and better bit error rate performance is achieved. An Extended Kalman filter is proposed for detection in [10] to mitigate the ISI. Deep learning schemes are also proposed to demodulate the received molecules, in [11], convolutional neural network is studied, and in [12], deep neural network is considered.

In DBMC, during the propagation of the released molecules, the molecules may be degraded due to the chemical reaction. In [13–15], the exponential degradation of the molecules during the propagation is considered. In [13], considering the molecular degradation, modulation schemes are proposed. In [16], the molecular degradation during the propagation and the molecular reaction with receiver receptor proteins is considered, and the expected received signal is analyzed. The results in [15] indicate that the degradation improves the system performance once appropriate select the degradation rate. Efficient deployment of the limited amount of enzymes in the channel to mitigate the ISI is studied in [17]. In [18], to mitigate the ISI, an enzymatic reaction is introduced by degrading the molecules in the channel.

In this paper, considering the degradation of the molecules in the channel, we propose a detection scheme based on maximum likelihood (ML). Though the ML detection scheme has been employed in the MC, however, in these schemes, molecular degradation is not considered, and molecular degradation is common in more practical MC systems. Therefore, in this paper, we first analyze the received signal considering molecular degradation during the propagation. Then, based on the received signal, a detection scheme based on the ML is conducted to mitigate the ISI. Finally, the simulations are performed to verify the effectiveness of the proposed scheme in the considered MC system.

The remainder of this paper is organized as follows. In Sect. 2, we discuss the considered MC system model with molecular degradation. In Sect. 3, we analyze the received signal and introduce the detection method based on the ML. In Sect. 4, we validate the ML detection method in the ISI mitigation with molecular degradation during the propagation. Finally, the conclusion of this paper is presented in Sect. 5.

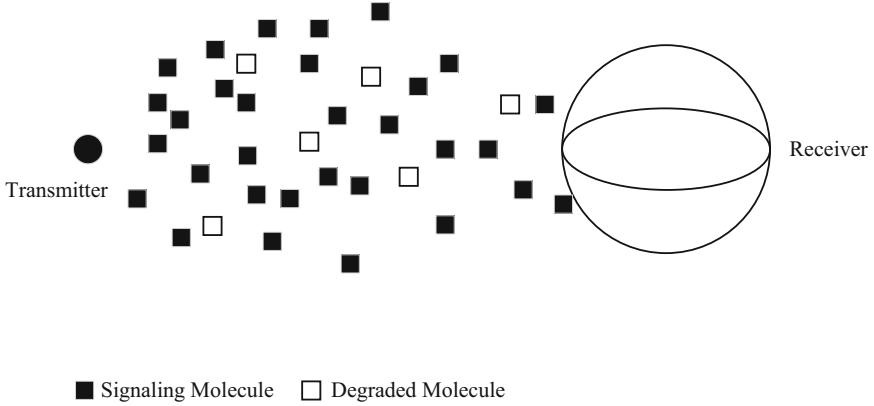


Fig. 1. The considered molecular communication system model.

2 System Model

In this paper, a three-dimensional (3D) MC system with a point transmitter and a sphere absorb receiver is considered. At the transmitter, the concentration shift keying (CSK) modulation scheme is employed, which indicates that to transmit bit 0, no molecule is released, while to transmit bit 1, N_m molecules are released. After the molecules are released from the transmitter, they propagate to the receiver by diffusion. Moreover, the exponential degradation of the molecules is taken into account during the propagation. The receiver detects and counts the number of received molecules. Then, based on the received signal, the received bits are demodulated by the ML detection method. The overall MC system model is shown in Fig. 1.

As shown in Fig. 1, the released molecules can be divided into two parts, one is the signaling molecules, which propagate in the channel and can be detected by the receiver. The other part is the degraded molecules, which are degraded in the channel before arriving at the receiver.

Considering the exponential decay degradation of the released molecules, assuming the initial concentration of released molecules is C_0 , then, at time t , the molecular concentration can be expressed as [15]

$$C(t) = C_0 e^{(-\lambda t)}, \quad (1)$$

where λ can be achieved by

$$\lambda = \frac{\ln 2}{\Lambda_{1/2}}, \quad (2)$$

where $\Lambda_{1/2}$ is the half lifetime of molecules.

Then, at time t , the fraction of absorbed molecules which are released at time $t = 0$ can be expressed as [15]

$$F(\lambda, t|r_0) = \frac{r_{rx}}{d + r_{rx}} \exp\left[-\sqrt{\frac{\lambda}{D}}d\right] - \frac{r_{rx}}{2(d + r_{rx})} e^{-\sqrt{\frac{\lambda}{D}}d} \times \left\{ \operatorname{erf}\left(\frac{d}{\sqrt{4Dt}} - \sqrt{\lambda t}\right) + e^{2\sqrt{\frac{\lambda}{D}}d} \times \left[\operatorname{erf}\left(\frac{d}{\sqrt{4Dt}} + \sqrt{\lambda t}\right) - 1 \right] + 1 \right\}, \quad (3)$$

where r_{rx} is the radius of the receiver, d is the distance between the transmitter and the receiver, and D is the diffusion coefficient of the molecules. During a bit interval T , the hitting probability can be expressed as

$$F_{\text{hit},1,\lambda} = F(\lambda, t + T|r_0) - F(\lambda, t|r_0). \quad (4)$$

For simple the notation, $F_{\text{hit},k-i+1,\lambda}$ denotes the hitting probability of molecules released at the beginning of i th bit interval and observed during the k th bit interval and considering the molecular degradation during the propagation. $F_{\text{hit},1,\lambda}$ denotes the hitting probability of molecules released at the beginning of the k th bit interval and observed during the k th bit interval.

Then, after N_m are released from the transmitter at time t_0 , the expected number of received molecules during a bit interval can be expressed as

$$\mathbb{E}[N_{rx,\lambda}] = N_m F_{\text{hit},1,\lambda}. \quad (5)$$

In DBMC, due to the channel memory, making the absorbed molecules at the receiver in a bit interval not only from the at the current bit interval but also from molecules released at the previous bit interval. Therefore, considering the channel memory, the received molecules in the k th bit interval can be expressed as

$$N_{rx,k,\lambda} = N_{rx,c,k,\lambda} + N_{rx,\text{ISI},k,\lambda} + N_{rx,n,k,\lambda}, \quad (6)$$

where $N_{rx,c,k,\lambda}$ denotes the molecules released at the beginning of k th bit interval and received during the k th bit interval; $N_{rx,\text{ISI},k,\lambda}$ is the molecules released from the previous bit interval but received during the k th bit interval; and $N_{rx,n,k,\lambda}$ is the counting noise.

After N_m molecules are released from the transmitter at the beginning of k th bit interval, the received molecules $N_{rx,c,k,\lambda}$ during the k th bit interval can be expressed as

$$N_{rx,c,k,\lambda} = N_m F_{\text{hit},1,\lambda}. \quad (7)$$

The $N_{rx,c,k,\lambda}$ can be approximated by the normal distribution and expressed as

$$N_{rx,c,k,\lambda} \sim \mathcal{N}(N_m F_{\text{hit},1,\lambda}, N_m F_{\text{hit},1,\lambda} (1 - F_{\text{hit},1,\lambda})). \quad (8)$$

The interference molecules $N_{rx,ISI,k,\lambda}$ can be expressed as

$$N_{rx,ISI,k,\lambda} = \sum_{i=1}^{k-1} \mathbb{N}_{rx,ISI,i,\lambda}, \quad (9)$$

where $\mathbb{N}_{rx,ISI,i,\lambda}$ denotes the molecules released at the beginning of i th bit interval but received during the k th bit interval and can be expressed as

$$\mathbb{N}_{rx,ISI,i,\lambda} = N_{tx,i} F_{hit,k-i+1,\lambda}, \quad (10)$$

where $N_{tx,i}$ denotes the number of transmitted molecules at the beginning of i th bit interval, and for bit 0, no molecule is released, while for bit 1, N_m molecules are released. The $\mathbb{N}_{rx,ISI,i,\lambda}$ can be approximated by the normal distribution

$$\mathbb{N}_{rx,ISI,i,\lambda} \sim \mathcal{N}(N_{tx,i} F_{hit,k-i+1,\lambda}, N_{tx,i} F_{hit,k-i+1,\lambda} (1 - F_{hit,k-i+1,\lambda})). \quad (11)$$

In DBMC, the counting noise $N_{rx,n,k,\lambda}$ is a random process of molecules entering/leaving the receptor space of the receiver and is usually assumed to follow a Gaussian distribution with 0 mean and the variance depends on the received molecules and can be expressed as

$$N_{rx,n,k,\lambda} \sim \mathcal{N}(0, \sigma_n^2). \quad (12)$$

3 Maximum Likelihood Detection Method

In this section, the ML detection scheme is employed at the receiver to detect the received bits and mitigate the ISI. Without loss of generality, we assume all the transmission bits are random and independent. Then, based on (7)–(12), the received molecules can be approximated by the normal distribution $N_{rx,k,\lambda} \sim \mathcal{N}(\mu_{rx,k,\lambda}, \sigma_{rx,k,\lambda}^2)$. Let H_0 be the hypothesis that bit 0 is transmitted; therefore, under H_0 , the mean $\mu_{0,k,\lambda}$ and variance $\sigma_{0,k,\lambda}^2$ of the received molecules can be expressed as

$$\mu_{0,k,\lambda} = \mu_{I,k,\lambda} + \mu_{n,k,\lambda} = \frac{1}{2} \sum_{i=1}^{k-1} N_{tx,i} F_{hit,k-i+1,\lambda}, \quad (13)$$

$$\begin{aligned} \sigma_{0,k,\lambda}^2 &= \sum_{i=1}^{k-1} \sigma_{I,j,\lambda}^2 + \sigma_{n,k,\lambda}^2 \\ &= \sum_{i=1}^{k-1} \left[\frac{1}{2} N_{tx,i} F_{hit,k-i+1,\lambda} (1 - F_{hit,k-i+1,\lambda}) + \frac{1}{4} (N_{tx,i} F_{hit,k-i+1,\lambda})^2 \right] + \mu_{0,k}. \end{aligned} \quad (14)$$

Let H_1 be the hypothesis that bit 1 is transmitted, therefore, under H_1 , the mean $\mu_{1,k,\lambda}$ and variance $\sigma_{1,k,\lambda}^2$ of the received molecules can be expressed as

$$\begin{aligned}\mu_{1,k,\lambda} &= \mu_{c,k,\lambda} + \mu_I,k,\lambda + \mu_n,k,\lambda \\ &= N_{tx,k} F_{\text{hit},1,\lambda} + \frac{1}{2} \sum_{i=1}^{k-1} N_{tx,i} F_{\text{hit},k-i+1,\lambda},\end{aligned}\quad (15)$$

$$\begin{aligned}\sigma_{1,k,\lambda}^2 &= \sigma_{c,k,\lambda}^2 + \sigma_I,k,\lambda^2 + \sigma_n,k,\lambda^2 \\ &= N_{tx,k} F_{\text{hit},1,\lambda} (1 - F_{\text{hit},1,\lambda}) + \sum_{i=1}^{k-1} \left[\frac{1}{2} N_{tx,i} F_{\text{hit},k-i+1,\lambda} (1 - F_{\text{hit},k-i+1,\lambda}) \right] \\ &\quad + \sum_{i=1}^{k-1} \left[\frac{1}{4} (N_{tx,i} F_{\text{hit},k-i+1,\lambda})^2 \right] + \mu_{1,k,\lambda}.\end{aligned}\quad (16)$$

The bit detection at the receiver in the k th bit interval by employing the ML decision rule can be expressed as

$$\hat{b}_{rx,k} = \arg \max_{b_{tx,k}} f(N_{rx,k,\lambda} | H_x), \quad (17)$$

where $b_{tx,k}$ is the transmitted bits sequence and $b_{tx,k} \in \{0, 1\}$, $f(N_{rx,k,\lambda} | H_x)$ denotes the conditional PDF of $N_{rx,k,\lambda}$ under the hypothesis H_x . Based on (13) and (14), the conditional PDF of $N_{rx,k,\lambda}$ under the hypothesis H_0 which assumes bit 0 is transmitted can be expressed as

$$f(N_{rx,k,\lambda} | H_0) = \frac{1}{\sqrt{2\pi\sigma_{0,k,\lambda}^2}} \exp\left(-\frac{(N_{\text{thr}} - \mu_{0,k,\lambda})^2}{2\sigma_{0,k,\lambda}^2}\right). \quad (18)$$

And Based on (15) and (16), the conditional PDF of $N_{rx,k,\lambda}$ under the hypothesis H_1 which assumes bit 1 is transmitted can be expressed as

$$f(N_{rx,k,\lambda} | H_1) = \frac{1}{\sqrt{2\pi\sigma_{1,k,\lambda}^2}} \exp\left(-\frac{(N_{\text{thr}} - \mu_{1,k,\lambda})^2}{2\sigma_{1,k,\lambda}^2}\right). \quad (19)$$

Therefore, the optimal detection threshold N_{thr} can be achieved by setting

$$\frac{1}{\sqrt{2\pi\sigma_{0,k,\lambda}^2}} \exp\left(-\frac{(N_{\text{thr}} - \mu_{0,k,\lambda})^2}{2\sigma_{0,k,\lambda}^2}\right) = \frac{1}{\sqrt{2\pi\sigma_{1,k,\lambda}^2}} \exp\left(-\frac{(N_{\text{thr}} - \mu_{1,k,\lambda})^2}{2\sigma_{1,k,\lambda}^2}\right), \quad (20)$$

Then the optimal detection threshold N_{thr} can be achieved as

$$N_{\text{thr}} = \frac{1}{\sigma_{1,k,\lambda}^2 - \sigma_{0,k,\lambda}^2} \left[(\mu_{0,k,\lambda}\sigma_{1,k,\lambda}^2 - \mu_{1,k,\lambda}\sigma_{0,k,\lambda}^2) + \sigma_{0,k,\lambda}\sigma_{1,k,\lambda} \sqrt{(\mu_{0,k,\lambda} - \mu_{1,k,\lambda})^2 + 2(\sigma_{1,k,\lambda}^2 - \sigma_{0,k,\lambda}^2) \ln \frac{\sigma_{1,k,\lambda}}{\sigma_{0,k,\lambda}}} \right]. \quad (21)$$

At the receiver, the bits are decoded according to the following rule

$$\hat{b}_{rx,k} = \begin{cases} 1, & N_{rx,k,\lambda} \geq N_{\text{thr}} \\ 0 & N_{rx,k,\lambda} < N_{\text{thr}}. \end{cases} \quad (22)$$

In DBMC, considering the channel memory, the error in the k th bit interval is not only related to the molecules transmitted in the current bit interval but also the previous bit interval. Therefore, the bit error rate can be expressed as

$$P_{e,k,\lambda} = \sum_{(b_{tx,1}, \dots, b_{tx,k}) \in \{0,1\}^k} \Pr(b_{tx,1}, \dots, b_{tx,k}) \Pr(\text{error} | b_{tx,1}, \dots, b_{tx,k}). \quad (23)$$

In DBMC, an error is occurred when the decoded bit not equal to the transmitted bit, namely $\hat{b}_{rx,k} \neq b_{tx,k}$. The error for transmitting bit 0 and bit 1 can be expressed as

$$\Pr(N_{rx,k,\lambda} > N_{\text{thr}} | b_{tx,k} = 0) = Q\left(\sqrt{\frac{(N_{\text{thr}} - \mu_{0,k,\lambda})^2}{\sigma_{0,k,\lambda}^2}}\right), \quad (24)$$

$$\Pr(N_{rx,k,\lambda} > N_{\text{thr}} | b_{tx,k} = 1) = Q\left(\sqrt{\frac{(N_{\text{thr}} - \mu_{1,k,\lambda})^2}{\sigma_{1,k,\lambda}^2}}\right). \quad (25)$$

Thus, the average bit error probability in the k th time slot for the same probability to transmit bit 0 and bit 1 can be expressed as

$$P_{e,k,\lambda} = \frac{1}{2} \left(1 - Q\left(\frac{N_{\text{thr}} - \mu_{1,k,\lambda}}{\sigma_{1,k,\lambda}}\right) \right) + \frac{1}{2} Q\left(\frac{N_{\text{thr}} - \mu_{0,k,\lambda}}{\sigma_{0,k,\lambda}}\right). \quad (26)$$

4 Numerical and Simulation Results

In this section, numerical and simulations are conducted to verify the effectiveness of the ML detection scheme in mitigating ISI in the DBMC system considering the degradation of the molecules during the propagation. The parameters are listed in Table 1.

In Fig. 2, the molecular concentration varies with time under the different half lifetime of molecules $\Lambda_{1/2}$ are compared. As shown in Fig. 2, the molecular concentration decreases with time, however, the decrease rate is affected by the half lifetime of molecules $\Lambda_{1/2}$. For the larger half lifetime of molecules $\Lambda_{1/2}$, the longer time the molecules propagate, therefore, more molecules are probability to be absorbed by the receiver, making the higher molecular concentration.

Table 1. Simulation parameters.

Simulation parameters	Symbol	Value
Distance between transmitter and receiver	d	$4 \mu\text{m}$
Radius of receiver	r_{rx}	$6 \mu\text{m}$
Diffusion coefficient	D	$79.4 \mu\text{m}^2/\text{s}$
Number of transmitter molecules for bit 1	N_{tx}	10000
Half-lifetime of released molecules	$\Lambda_{1/2}$	0.128 s, 0.064 s, 0.032 s
Bit interval	T	0.5 s

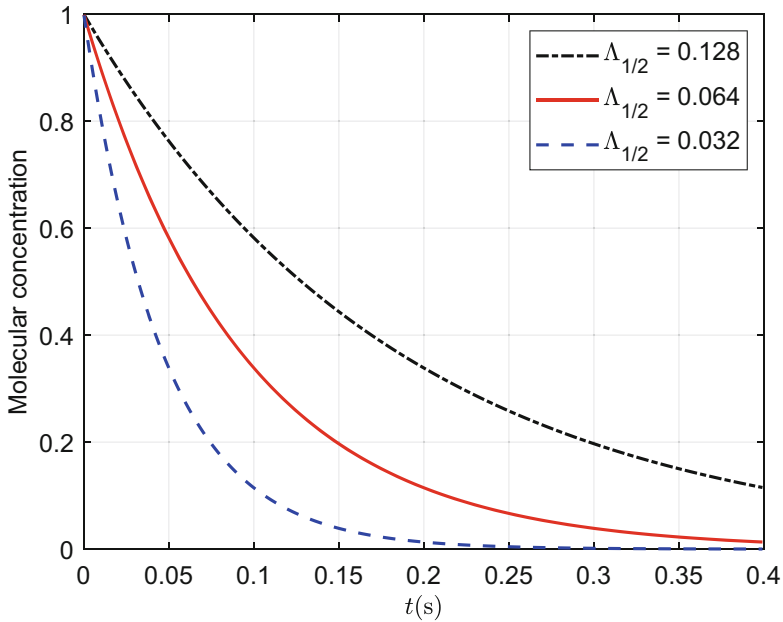
**Fig. 2.** The molecular concentration varies with time t . The initial molecular concentration $C_0=1$.

Figure 3 illustrates the fraction of molecules absorbed by the receiver varies with time under the different half lifetime of molecules $\Lambda_{1/2}$. It can be clearly seen from Fig. 3, for the larger half lifetime of molecules $\Lambda_{1/2}$, the higher fraction of molecules absorbed by the receiver due to the larger half lifetime of molecules $\Lambda_{1/2}$, the longer lifetime of the molecules, then, making more molecules are absorbed by the receiver.

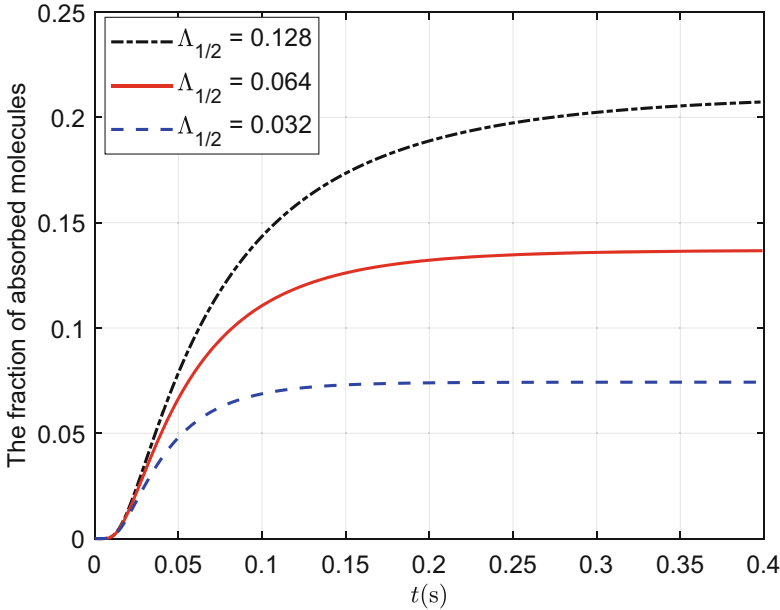


Fig. 3. The fraction of absorbed molecules varies with time t .

In Fig. 4, we illustrate the BER varies with the detection threshold under the different half lifetime of molecules $\Lambda_{1/2}$. It is shown in Fig. 4, for the smaller half lifetime of molecules $\Lambda_{1/2}$, the optimal detection threshold is smaller, and it achieves better BER performance. This is because, for the smaller $\Lambda_{1/2}$, more molecules are degraded during the propagation, therefore, fewer molecules remain in the channel, and this decreases the effect for future transmission. So, for the smaller half lifetime of molecules $\Lambda_{1/2}$, the optimal detection threshold is also smaller, and it achieves better BER performance.

In Fig. 5, we illustrate the BER varies with SNR under the different half lifetime of molecules $\Lambda_{1/2}$ based on the ML detection. As shown in Fig. 5, with the increase of SNR, the BER decreases, and the BER is also affected by the $\Lambda_{1/2}$. For the smaller $\Lambda_{1/2}$, it achieves better BER performance, due to the smaller $\Lambda_{1/2}$, the molecules degrade during the propagation and there are fewer molecules remaining in the channel namely lower ISI. It also verified the effectiveness of ML detection in the DBMC system with molecular degradation during the propagation.

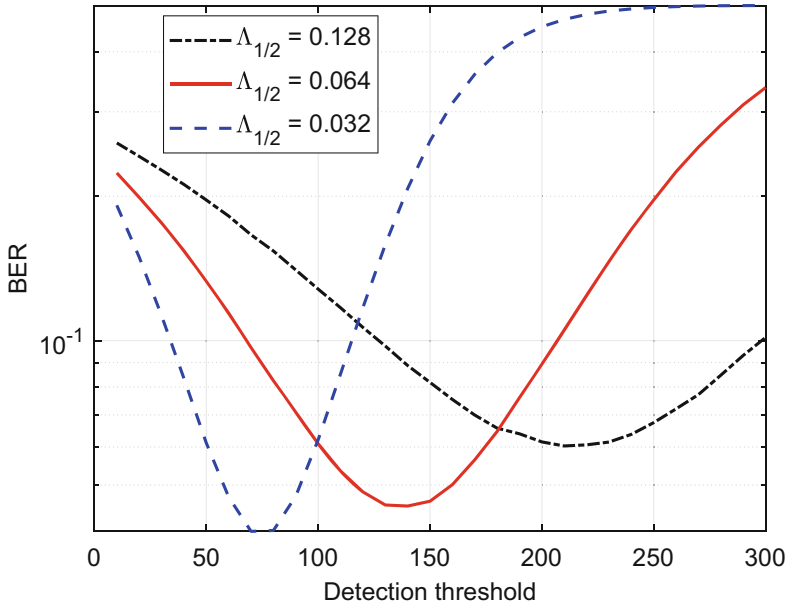


Fig. 4. The BER varies with the detection threshold.

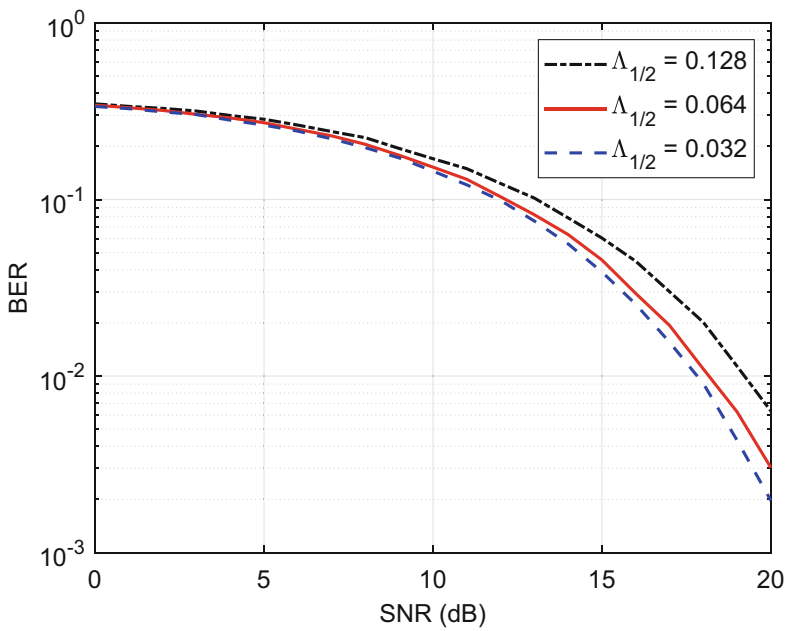


Fig. 5. The BER varies with SNR in the considered DBMC.

5 Conclusion

In this paper, we considered a DBMC system in which the released molecules degrade during propagation. Considering the degradation of molecules during the propagation, the received molecules are analyzed. Then, based on the mean and variance of the received molecules, the ML detection method is employed to detect the received bits and mitigate the ISI. Simulation results verified the effectiveness of the ML detection method in the ISI mitigation in the DBMC system when the degradation of the molecule during the propagation is considered.

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