

# Optimal Detection for Diffusion-Based Communications in the Presence of ISI

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**Abstract**—Communications based on diffusion refers to the transfer of information using molecules as message carriers whose propagation is governed by the laws of Brownian motion. Molecular communication is considered to be one of the most promising approaches for the end-to-end communication between nanoscale devices. In this paper, both an optimal and a suboptimal receiver detection scheme are proposed for a diffusion-based binary digital communication system in the presence of ISI. The transmission of binary information is accomplished by using On-Off Keying (OOK) with only one molecule. The proposed system can serve as the theoretical basis for end-to-end communication in molecular nanonetworks where molecules of different types are used by different nanoscale devices. The effect of channel memory resulting from the residual molecule diffusion from previous transmissions is treated analytically in the formulation of the detection schemes. Numerical results show that the proposed detection schemes can maximize the mutual information over a practical range of the parameter of signaling interval without *a priori* information. A channel capacity of 1 bit per channel utilization during a signaling interval can be ultimately achieved by extending the duration of the signaling interval, even with infinite channel memory.

**Index Terms**—Molecular communication, diffusion process, Brownian motion, Neyman-Pearson criterion, mutual information, channel capacity

## I. INTRODUCTION

Nanotechnology has seen dramatic progress in its development over the past few years [1]. A nanomachine is a device which is envisioned to perform a specific task, e.g., processing, sensing and actuation, and can be considered as the most basic unit [2]. Molecular communication, defined as the transfer of information using molecules as message carriers, has been shown to be one of the most promising solutions for communications between nanomachines. Molecular communication based on *diffusion* refers to the situation where molecules reach the destination relying solely on the laws of molecular diffusion.

Based on the types of molecules, we envision two different approaches for characterizing *nanonetworks* with molecular communication, namely *homogeneous* and *heterogeneous* molecular nanonetworks. In the homogeneous case, the information molecules are all the same (i.e., indistinguishable).

An obvious advantage is the simplicity of generating information molecules by nanomachines since only a single type of molecule must be synthesized. However, the effect of Multi-User Interference (MUI) arises due to the fact that the nanomachine at the receiving end has no knowledge whether the molecules were emitted from the intended transmitting nanomachine or from any other interfering sources, which complicates the design of the signaling and detection schemes. In the heterogeneous case, the information molecules are distinguishable for distinct communication channels such that *orthogonal molecular communication* can be achieved [3]. The cost and complexity of synthesizing the information molecules in this case is expected to be higher when compared with the homogeneous case. However, the signaling and detection schemes can be largely simplified since the effect of MUI is inherently nonexistent. As nanomachines are very limited in functionality, the heterogeneous approach seems to be more promising if the added overhead of synthesizing molecules is justified by the simplicity of the signaling schemes.

A thorough investigation of the end-to-end communication mechanism between nanomachines is required before the molecular nanonetworks can be practically considered. Borrowing from the paradigm of traditional ElectroMagnetic (EM) communications, molecular communication systems using digital signaling, e.g., binary signaling and multi-amplitude signaling, are emerging and drawing increasing attention [5]–[12]. It has been indicated that the effect of channel memory, hence Inter-Symbol Interference (ISI), resulting from the residual molecule diffusion from previous transmissions in diffusion-based digital communication is critically important [6], [8]. However, simplified channel models and receiver design without mathematical foundations are assumed for making the analysis tractable. For example, a diffusion channel with limited orders of memory is assumed in [10]–[12]. Stochastic degradation of the information molecules is considered using simulations in [7]. Heuristic decision rules where the detection threshold is not mathematically obtained are considered in [9]–[12]. Such simplified channel model and heuristic detection approaches raise the concern of the feasibility of diffusion-based communication systems in the

presence of large or even infinite channel memory.

In this paper, we propose the design of a diffusion-based communication system for transmission of binary digital information, which is accomplished by using On-Off Keying (OOK) with only one molecule. The proposed system can serve as the theoretical basis for end-to-end communication in heterogeneous molecular nanonetworks. By adopting an information-theoretic approach, the optimal detection strategy is formulated with arbitrary orders of channel memory. Specifically, we propose a one-shot detector with two detection schemes for mutual information maximization: an information-optimal detection scheme with perfect *a priori* information and a suboptimal detection scheme without *a priori* information. To the best of the authors' knowledge, this is the first work that gives an analytical treatment of the optimal detection problem for diffusion-based communication in the presence of ISI. Numerical results indicate that the *a priori* information is not needed, and the proposed suboptimal detection scheme can achieve optimal detection performance over a practical range of the parameter of signaling interval. Also, it is shown that our receiver design guarantees diffusion-based communication to operate without failure even in the case of infinite channel memory. A channel capacity of 1 bit per channel utilization during a signaling interval can be ultimately achieved by extending the duration of the signaling interval.

The rest of this paper is organized as follows. In Section II, we introduce the system model of the proposed communication system based on diffusion. In Section III, we propose our design of the digital receiver and develop the detection schemes using an information-theoretic approach. In Section IV, the numerical results are presented. Finally, conclusions are given in Section V.

## II. SYSTEM MODEL

We propose a time-slotted system with signaling interval  $T_s$  in a one-dimensional diffusion space. In this paper, we assume perfect synchronization between the transmitter and the receiver. With *a priori* probability  $p$ , a single molecule is emitted by the transmitter at the beginning of each signaling interval to signify logical 1; no molecule is emitted to signify 0. The molecule moves toward one of the two ends of the diffusion space by an infinitesimal length with equal probability, which results in a one-dimensional random walk of the molecule from the transmitter to the receiver. We assume this random walk stops once the molecule reaches the receiver. Let  $T$  denote the random variable representing the first hitting time of the molecule at the receiver side. This random variable is the result of a random process which is described by the Brownian motion. As a consequence, the cumulative distribution function (c.d.f) of  $T$  is [13]

$$F(t) = \frac{2}{\sqrt{2\pi}} \int_{\frac{r}{\sqrt{2Dt}}}^{\infty} e^{-y^2/2} dy = 2Q\left(\frac{r}{\sqrt{2Dt}}\right), \quad (1)$$

where  $r$  denotes the distance between the transmitter and the receiver,  $D$  is the diffusion constant, and  $Q(\cdot)$  is the standard Q-function defined as  $Q(x) = \frac{1}{\sqrt{2\pi}} \int_x^{\infty} e^{-y^2/2} dy$ .

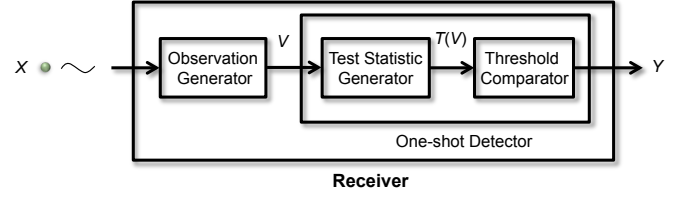


Fig. 1. High-level scheme of the proposed digital receiver.

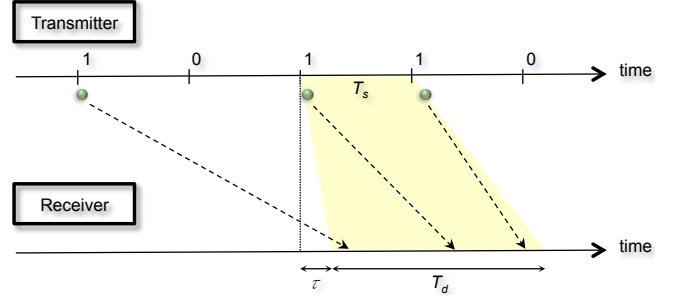


Fig. 2. Illustration of the molecule counter. In this example, the intended information is 1, and we have  $V = 3$ .

Due to the uncertainty lying in the hitting time  $T$  of the molecule following the Brownian motion, channel memory arises as the transmitted molecules stay in the diffusion channel for an indefinite period of time, which leads to Inter-Symbol Interference (ISI). In the following, we denote the number of interfering signaling intervals by  $N$ .

## III. RECEIVER DESIGN

We propose a high-level scheme for modeling the receiver in the proposed molecular communication system as in Fig. 1. The *observation generator* generates a quantitative description  $V$  of the binary information  $X$  sent in the current signaling interval  $T_s$  based on a certain measurable characteristic of the arriving molecules, e.g., the accumulated number of arriving molecules and the time of arrivals. For the detector design, we propose a one-shot detection approach which only utilizes information in the corresponding decision duration  $T_d$ , which in general, can be different from the signaling interval  $T_s$ . The *test statistic generator* computes a test statistic, denoted by  $T(V)$ , based on the quantitative description  $V$ . It is demonstrated in Section IV that the proposed detection scheme with  $T(V) = V$  achieves maximum mutual information over a wide range of system parameters, and it is particularly well-suited for low-end nano-devices. The *threshold comparator* compares the test statistic  $T(V)$  with a predetermined threshold to generate the binary decision  $Y$ .

We remark that a sequence detector, e.g., a Maximum Likelihood (ML) detector, can also be employed in place of the one-shot detector by jointly deciding on a sequence of transmitted binary information based on the corresponding sequence of observations. The tradeoff between the performance boost and the computational complexity, however, must take into account the limited capabilities of nanoscale devices. The study of such an issue should be based on top of the proposed detection framework, and it is out of the scope of this paper.

### A. Observation Generator

In this work, we consider the observation generator as a molecule counter. The molecule counter counts the total number of molecules hitting the receiver within a predetermined decision duration, denoted by  $T_d$ . As demonstrated in Section IV, the setting of  $T_d$  is to be optimized and is not necessarily equal to  $T_s$ . A predetermined delay  $\tau$  is applied to account for the propagation delay. Note that if  $T_d + \tau > T_s$ , interference from the following signaling intervals also arises since the molecules emitted in the the following signaling intervals could fall into the current decision duration  $T_d$ . Fig. 2 provides an illustration of the molecule counter.

For a given value of  $T_d$ , we propose to apply a predetermined delay  $\tau$  which maximizes the probability that the emitted molecule falls into the decision duration. This is expressed as follows

$$\begin{aligned}\tau &= \operatorname{argmax}_{\tilde{\tau}} P(\tilde{\tau} \leq T < T_d + \tilde{\tau}) \\ &= \operatorname{argmax}_{\tilde{\tau}} F(T_d + \tilde{\tau}) - F(\tilde{\tau}).\end{aligned}\quad (2)$$

By applying (1) to (2), and after some manipulations, we obtain the following equation in the variable  $\tau$

$$\exp\left(-\frac{r^2 T_d}{2D\tau(T_d + \tau)}\right) - \left(\frac{\tau}{T_d + \tau}\right)^3 = 0, \quad (3)$$

which can be computed numerically.

### B. Detector

Since there is no assumption of any favorable value for the *a priori* probability  $p$  for binary signaling or a proper definition of Bayesian cost [14] for a diffusion-based communication channel, we adopt an information-theoretic approach. According to this approach, the ultimate goal of the detector design is concerned with the following optimization problem

$$\max I(X; Y), \quad (4)$$

where  $I(\cdot)$  refers to the mutual information, which is defined as follows [14]

$$I(X; Y) = \sum_{x=0}^1 \sum_{y=0}^1 P(Y|X)P(X) \log \frac{P(Y|X)}{P(Y)}. \quad (5)$$

By definition, we have

$$\begin{aligned}P(Y = 1 | X = 0) &= P_F, \\ P(Y = 1 | X = 1) &= P_D, \\ P(Y = 0 | X = 0) &= 1 - P_F, \\ P(Y = 0 | X = 1) &= 1 - P_D,\end{aligned}\quad (6)$$

where  $P_F$  and  $P_D$  denote the false alarm probability and the detection probability, respectively. The mutual information is therefore a function of  $P_F$ ,  $P_D$ , and the *a priori* probability  $P(X = 1) = p$ . We henceforth denote the mutual information by  $I(P_F, P_D, p)$ . It is shown in [15] that given  $P_F$ , the mutual information is a monotonically increasing function of  $P_D$ . Thus an information-optimal detector which maximizes the mutual information is equivalent to a Neyman-Pearson

detector [16] when  $P_F$  is given. In the following, we first formulate the binary hypothesis testing problem and then apply the Neyman-Pearson decision rule to derive the optimal detection scheme, including the corresponding test statistic and the decision threshold.

1) *Detection with Perfect A Priori Information*: First we consider the case where the receiver has perfect knowledge of the *a priori* probability  $p$ . The detector is concerned with the binary hypothesis testing problem

$$\begin{aligned}H_1: & \text{a molecule is emitted at } t = 0; V \sim P_V^1(v), \\ H_0: & \text{otherwise; } V \sim P_V^0(v),\end{aligned}\quad (7)$$

where  $P_V^k(v)$  denotes the probability mass function of  $V$  given that hypothesis  $H_k$  is true. To characterize the probability distribution of  $V$ , let  $W_j$  denote the random variable which is defined as the event in which the molecule from the  $j$ -th previous signaling interval arrives within the current decision duration  $[\tau, T_d + \tau)$ .  $W_j$  represents the ISI component from the  $j$ -th previous signaling interval, with the exception of  $j = 0$  being the event concerning the arrival of the intended information molecule from the current signaling interval in the current decision duration. It is clear that  $W_j$  is a Bernoulli random variable with success probability

$$p_s^j = p \cdot (F(jT_s + T_d + \tau) - F(jT_s + \tau)), \quad (8)$$

where  $j = 0, \dots, N$ . In the case that  $T_d + \tau > T_s$ , and hence interference from the following signaling intervals arises, we define  $K = \lfloor \frac{T_d + \tau}{T_s} \rfloor$ , and  $W_l$  as a Bernoulli random variable with success probability

$$p_s^l = p \cdot (F(T_d + \tau - (l-N)T_s) - F(\max\{\tau - (l-N)T_s, 0\})), \quad (9)$$

where  $l = N+1, \dots, N+K$ .  $W_l$  represents the ISI component from the  $(l-N)$ -th following signaling interval. Due to the properties of the Brownian motion [17], the molecules arriving from different signaling intervals are independent. We can thus express  $V$  as a sum of independent non-identically distributed Bernoulli trials

$$\begin{aligned}P_V^1(v) &= W_0 + \sum_{j=1}^N W_j + \sum_{l=N+1}^{N+K} W_l, \\ P_V^0(v) &= \sum_{j=1}^N W_j + \sum_{l=N+1}^{N+K} W_l,\end{aligned}\quad (10)$$

where  $\sum_{j=1}^N W_j + \sum_{l=N+1}^{N+K} W_l$  represents the aggregate effect of the ISI. In this case, the probabilities can be computed in an iterative fashion as [18]

$$P_V^1(v) = \frac{1}{v} \sum_{j=0}^{N+K} p_s^j P_{N+K}^1(v-1; j), \quad (11)$$

where  $v = 1, \dots, N+K+1$ , and  $P_{N+K}^1(v-1; j)$  is defined as the probability of  $v-1$  successes from the  $N+K$  trials excluding the  $j$ -th trial. For  $v = 0$ , it is straightforward that  $P_V^1(0) = \prod_{j=0}^{N+K} (1 - p_s^j)$ .  $P_V^0(v)$  can be computed in a similar fashion.

The Neyman-Pearson decision criterion states that the constrained optimization problem of maximizing  $P_D$  given a maximum allowable  $P_F$  is solved by formulating the likelihood ratio test [19]

$$\begin{cases} 1, & \text{if } \Lambda(v) > \lambda, \\ \rho, & \text{if } \Lambda(v) = \lambda, \\ 0, & \text{if } \Lambda(v) < \lambda. \end{cases} \quad (12)$$

where  $\Lambda(v) = \frac{P_V^1(v)}{P_V^0(v)}$ , and  $\rho$  stands for a randomized decision such that it is equal to hypothesis  $H_1$  with probability  $\rho$ .  $\lambda$  and  $\rho$  are determined by first finding  $\tilde{v}$  such that

$$0 \leq P_F - \sum_{\forall v, \Lambda(v) > \Lambda(\tilde{v})} P_V^0(v) < \sum_{\forall v, \Lambda(v) = \Lambda(\tilde{v})} P_V^0(v). \quad (13)$$

We then have

$$\begin{aligned} \lambda &= \Lambda(\tilde{v}), \\ \rho &= \frac{P_F - \sum_{\forall v, \Lambda(v) > \Lambda(\tilde{v})} P_V^0(v)}{\sum_{\forall v, \Lambda(v) = \Lambda(\tilde{v})} P_V^0(v)}. \end{aligned} \quad (14)$$

The corresponding  $P_D$  is then

$$P_D(P_F) = \sum_{\forall v, \Lambda(v) > \lambda} P_V^1(v) + \rho \sum_{\forall v, \Lambda(v) = \lambda} P_V^1(v). \quad (15)$$

Note we consider  $P_D$  as a function of  $P_F$ ,  $P_D(P_F)$ , as  $P_D$  is uniquely determined by  $P_F$  after applying the Neyman-Pearson decision rule [16].

To formulate the optimal detection scheme, it remains to find the optimal value of  $P_F$  which yields the maximum mutual information given the knowledge of the *a priori* probability  $p$ . This is expressed as follows

$$P_F^*(p) = \operatorname{argmax}_{P_F} I(P_F, P_D(P_F), p). \quad (16)$$

By using (13) and (14), we can obtain the corresponding information-optimal decision thresholds  $\lambda^*(p)$  and  $\rho^*(p)$ . It thus follows that an information-optimal test statistic generator is  $T(V) = \Lambda(V)$ , and the threshold comparator policy is given in (12) when  $\lambda^*(p)$  and  $\rho^*(p)$  are applied.

In the case where the receiver has control over the *a priori* probability  $p$ , e.g., by affecting the coding scheme, it is straightforward that the optimal value is determined such that the mutual information is further maximized over all possible values of  $p$  as

$$p^* = \operatorname{argmax}_p I(P_F^*(p), P_D(P_F^*(p)), p). \quad (17)$$

Note that the corresponding maximum mutual information  $I(P_F^*(p^*), P_D(P_F^*(p^*)), p^*)$  represents the theoretically maximum achievable information rate of the considered molecular communication system instead of the channel capacity, since a specific modulation technique and channel observation are considered in this paper.

2) *Detection without A Priori Information*: In the case where the receiver has no information of the *a priori* probability, the concept of *minimax* [19] which tries to mitigate the worst possible situation, i.e., maximizing the mutual information at the *a priori* probability which yields the lowest mutual information, should be applied. However, as discussed in [15], the fact that  $I(P_F, P_D, p) = 0$  when  $p = 0$  or  $1$  renders the approach of minimax inappropriate. Alternatively, we apply a suboptimal threshold detection method which operates directly on the number of hitting molecules, i.e.,  $T(V) = V$ , and

$$\begin{cases} 1, & \text{if } V \geq \eta, \\ 0, & \text{if } V < \eta. \end{cases} \quad (18)$$

where  $\eta$  denotes the threshold on the number of hitting molecules for discriminating logical 1 from 0. It is straightforward that given the threshold  $\eta$ ,  $P_F$  and  $P_D$  are obtained as

$$\begin{aligned} P_F(\eta) &= \sum_{v=\eta}^{N+K} P_V^0(v), \\ P_D(\eta) &= \sum_{v=\eta}^{N+K+1} P_V^1(v). \end{aligned} \quad (19)$$

We propose the use of a decision threshold  $\eta^\dagger$  such that

$$\eta^\dagger = \operatorname{argmax}_\eta \int I(P_F(\eta), P_D(\eta), p) dp. \quad (20)$$

The setting of the threshold  $\eta^\dagger$  thus maximizes the integrated information amount and it is independent of the actual *a priori* probability  $p$ .

#### IV. NUMERICAL RESULTS

In this section, we present numerical results for the attainable mutual information of the molecular communication system by applying the proposed detection schemes. We adopt typical parameters for short-range molecular communication, which happens naturally as the mechanism for biochemical signaling in living cells, e.g., calcium ion signaling [4] and neural signaling [20]. In the following, we set the diffusion constant  $D = 10^{-6}$  cm<sup>2</sup>/s, the communication distance  $r = 20$   $\mu$ m. Unless otherwise stated, we set the number of interfering signaling intervals  $N = 50$ . Note that the parameter  $K$  is dependent on the adopted settings of the delay  $\tau$  and the decision duration  $T_d$ .

In Fig. 3, we plot the attainable mutual information of the proposed communication system by using the information-optimal detection with perfect *a priori* probability. Two sets of results which correspond to  $T_s = 1$  s and  $T_s = 8$  s are provided. For each set of results, we plot three curves for different settings of the decision duration:  $T_d = T_s$ ,  $T_d = 2T_s$ , and  $T_d = \frac{T_s}{2}$ . The circles indicate the points which achieve the channel capacity of the system as given in (17). We observe that higher mutual information can be achieved with longer signaling interval as one would expect due to a lower ISI. For the case that  $T_s = 8$  s, the setting of  $T_d = T_s$  yields the best performance out of the three; while the setting of  $T_d = 2T_s$  yields the best performance for the set of results with shorter

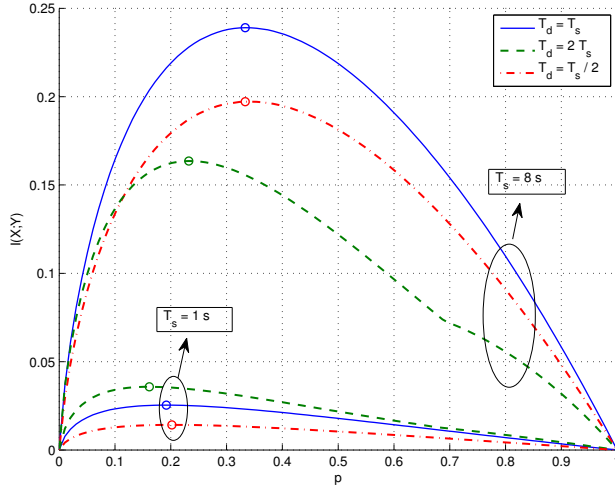


Fig. 3. Attainable mutual information versus the *a priori* probability  $p$  for different observation intervals using the optimal detection method. The circles indicate the points which achieve the maximum mutual information.

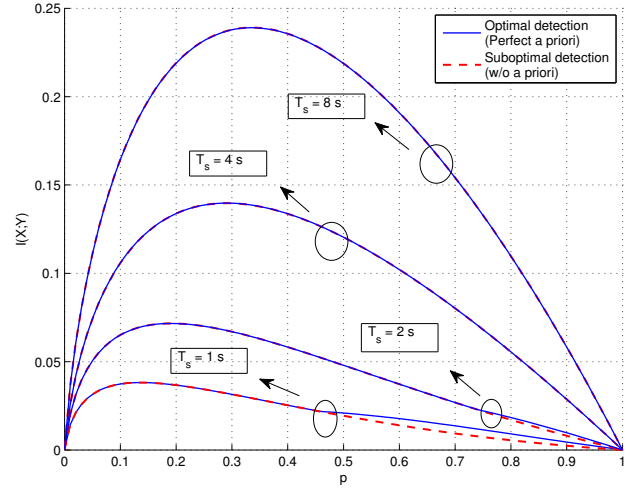


Fig. 5. Comparison between the attainable mutual information by using the optimal detection method and the suboptimal detection method. The optimal  $T_d$  is applied.

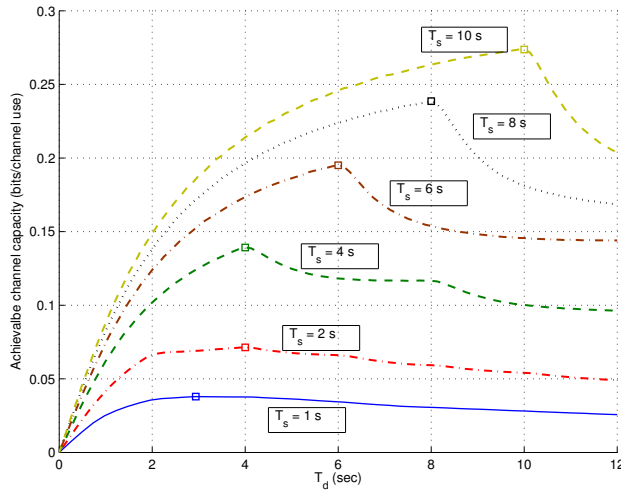


Fig. 4. Attainable channel capacity versus the decision duration  $T_d$  using the optimal detection method. The squares indicate the points which achieve the maximum channel capacity.

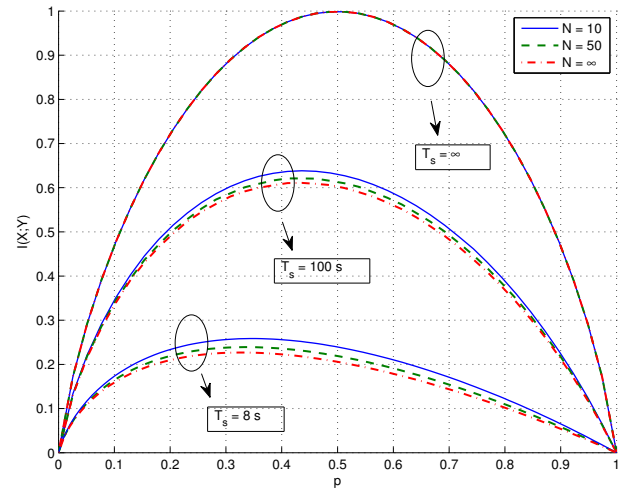


Fig. 6. Attainable mutual information versus the *a priori* probability  $p$  with different degrees of channel memory using the suboptimal detection method.  $T_d = T_s$ .

signaling interval. This suggests that the optimal value for the decision duration  $T_d$  is dependent on the signaling interval, and a relatively longer decision duration is desirable when the effect of ISI is more prominent. Finally, we observe that the system achieves the channel capacity at  $p < \frac{1}{2}$ . This is expected as fewer molecules cause less ISI, which in turn raises the mutual information.

In Fig. 4, we experiment with the optimal value for the decision duration and plot the attainable channel capacity as a function of the decision duration  $T_d$ . The information-optimal detection with perfect *a priori* probability is applied. The squares indicate the points which achieve the maximum channel capacity over all possible values of  $T_d$ . We again observe that a relatively long  $T_d$  is favorable when a short  $T_s$  is adopted. For  $T_s \geq 4$  s, the results indicate that the optimal

setting of  $T_d$  is consistently equal to  $T_s$ . Since it is not of practical interest to consider the case where  $T_s < 4$  s due to the strong ISI and hence low channel capacity, we conclude that the setting of  $T_d = T_s$  is optimal for all values of  $T_s$  which are of practical interest.

In Fig. 5, we compare the information-optimal detection (perfect knowledge of  $p$ ) with the proposed suboptimal detection without *a priori* information. The optimal  $T_d$  derived from Fig. 4 is applied here. We observe that by applying the proposed suboptimal detection scheme, the penalty of not knowing  $p$  only exists for small values of  $T_s$ . For values of  $T_s$  of practical interest, the two detection schemes yield identical performance. It is also worth noting that the detection threshold  $\eta^\dagger$  given in (20) is equal to 1 for all values of  $T_s$  considered here. Such result is satisfactorily intuitive as

there is one molecule emitted per signaling interval. We thus conclude that the proposed suboptimal detection scheme is information-optimal for all values of  $T_s$  of practical interest without the need of the *a priori* information.

In Fig. 6, we plot the attainable capacity with varying degrees of channel memory:  $N = 10$ ,  $N = 50$ , and  $N = \infty$ . Three sets of results are provided corresponding to different lengths of signaling intervals:  $T_s = 8$ ,  $T_s = 100$ , and  $T_s = \infty$ . Following the conclusions drawn from the previous results, we set  $T_d = T_s$  and employ the proposed suboptimal detection scheme. We observe that the attainable mutual information decreases by a small amount with increasing  $N$  due to the inclusion of more ISI, except for the case in which  $T_s = \infty$  where all three curves overlap. The results suggest that the analytical system performance with  $N = 50$  is very close to the case where there is infinite channel memory. More important, a channel capacity of 1 bit per channel utilization can be ultimately achieved with all degrees of channel memory by extending the duration of the signaling interval.

## V. CONCLUSIONS

In this paper, we have proposed the design of a digital molecular communication system based on diffusion along with an optimal receiver detection scheme. Binary digital signaling is accomplished by using OOK with only one single molecule in each signaling interval. The effect of channel memory resulting from the residual molecule diffusion has been considered and analyzed. The general framework for constructing the receiver as well as two detection schemes for mutual information maximization based on the availability of the *a priori* probability have been proposed. Numerical results indicate that the *a priori* probability is not needed to achieve the optimal detection performance, and the proposed suboptimal detection scheme can achieve the optimal detection performance over a practical range of the parameter of signaling interval. Also, it is shown that our receiver design guarantees diffusion-based communication to operate without failure even in the case of infinite channel memory. A channel capacity of 1 bit per channel utilization during a signaling interval can be ultimately achieved by extending the duration of the signaling interval.

By proposing and analyzing the binary digital communication system based on diffusion, we have devised a framework under which different signaling methods and detection schemes can be studied. A well-defined noise model as well as mutli-amplitude digital signaling schemes will be included in our future work. Such a framework also serves as the theoretical basis for our future study of various nanonetworking behaviors based on molecular communication.

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