On the Optimal Timing of Detection in Molecular Communication Systems

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***Abstract*—In this paper, the error performance of a molecular communication via diffusion system in the absence of flow is analysed. Closed-form expressions for the bit error rate are presented and utilized to enhance the timing of the receiver's observations, which are used in the detection of the transmitted information. More precisely, we specify the optimal time, when the observation process should start and finish, in order to achieve the minimum probability of error. Furthermore, in the case where the receiver counts the molecules at specific time instants, an advantageous sampling time has been proposed, along with the ideal number of samples that should be collected in order to minimize the error probability. Finally, closed-form expressions for the first sample and the total number of samples that should be considered, have been derived and validated through extensive simulations.**

***Index Terms*—Active receiver, amplitude detection, energy detection, molecular communication, passive receiver, sampling interval, sampling time, single threshold detection.**

I. Introduction

Nanotechnology is a scientific field with achievements that have given rise to various new needs, including the communication between nanoscale devices. Inspired by biological mechanisms, molecular communication (MC) utilizes molecules for the transfer of information between nanomachines [1], [2]. In this case, information carrying molecules diffuse freely and randomly in the communication medium and arrive at the receiver in a probabilistic manner. They may also reach the receiver at a later time than expected, thus creating intersymbol interference [3]. Besides, MC systems suffer from external noise, when molecules of the same type as the information carrying ones exist in the communication environment [3].

One of the challenges in MC is the design of reliable receivers of the least possible complexity. Depending on the requirements and the constraints of the considered application, different types of receivers can be utilized from one of the two main categories: a) those that interact with the molecules which enter their volume, i.e., *active receivers* [2], [4], and b) those that do not react with the molecules reaching their surface, i.e., *passive receivers* [3], [5]. The receivers of the first case can detect the transmitted information after counting the number of molecules received within a given time interval through *energy detection* [5]. Meanwhile, passive receivers can detect the information by counting the number of received molecules in predefined time instances, which is referred to as *amplitude detection with sampling* [3], [5].

In this paper, a diffusion-based MC system with either an active receiver employing energy detection or a passive receiver employing amplitude detection with sampling, is analyzed. Moreover, closed-form expressions for the system error probability are provided and utilized in order to select the optimal timing for the receiver's observations. To the best of the authors' knowledge, [6], [7] are the only works dealing with timing in MC systems. Nevertheless, they are both in a different context, focusing only on variable time symbol duration and not on the timing of the observations made at the receiver. The contribution of this paper can be summarized into the following two main points:

1) In the case of energy detection, the beginning and the end of the time interval, where the observations take place, are optimized, in order to decrease the error probability.
2) In the case of amplitude detection, a sampling time different from the commonly used in the literature [3] is proposed. Moreover, we manage to enhance the performance of MC systems in terms of error probability by providing the optimal number of samples that should be taken at the receiver along with the time instants when the sampling process should begin and end.

II. System Model

We consider a molecular communication system, consisting of a transmitter-receiver pair exchanging information via molecules of a certain type. The information to be transmitted is modulated via the number of molecules emitted instantaneously by the transmitter at the beginning of the symbol duration T. Perfect time synchronization is assumed between the transmitter and the receiver and ON/OFF keying modulation, implying that the emission of M molecules corresponds to bit-1 and no emission (i.e., zero molecules) to bit-0. The receiver is capable of identifying the specific type of the transmitted molecules.

As shown in Fig. 1, the transmitter is zero-dimensional, placed at a distance d from the closest point of the receiver's

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surface, which is considered spherical with radius r. The receiver works either as a passive or active observer. As has been already mentioned above, passive receivers do not interact with the molecules that collide with their surface, whereas active or absorbing receivers interact with the received molecules and fully absorb them, i.e., the molecules are removed from the communication environment. We assume that the receiver has the ability to count the number of observed molecules at any given time instant or interval and based on that it performs proper threshold detection.

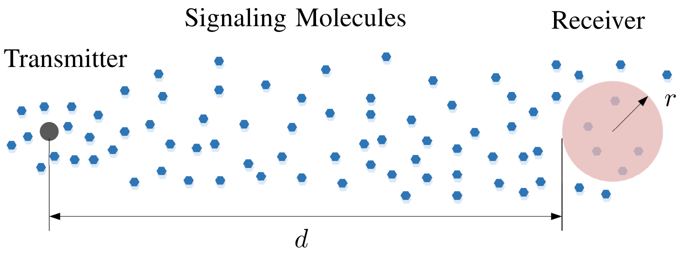

Fig. 1. Molecular communication system via diffusion.

Regarding the communication environment, it is assumed to be three-dimensional, stationary and unbounded in all dimensions, being filled with a fluid of uniform temperature and certain viscosity. The molecules diffuse freely towards all directions after their emission and propagate with Brownian motion. The motion of each molecule is considered to be independent of each other and affected by the diffusion coefficient D, which is constant and identical for all molecules. The molecules arrive at the receiver in a probabilistic manner due to their stochastic movement in the communication fluid. Therefore, the number of observed molecules within the receiver is a random variable (RV) following Poisson distribution with a proper mean value [3].

Besides, *external noise* is also present in the communication environment in the form of molecules that are of the same type as the information carrying ones. These noise molecules collide with the surface of the receiver, where they are mistaken as information carrying molecules, thus acting as additive noise to the observations. Finally, the considered system suffers from *intersymbol interference* (ISI) due to the fact that information molecules corresponding to a previous transmission may reach the receiver at a later time.

Next, the symbol duration, T, is defined as

$$T = \frac{b^2}{4D[\operatorname{erfc}^{-1}(\alpha)]^2}, \tag{1}$$

where $\operatorname{erfc}(\cdot)$ is the complementary error function, $b = d$ for the active receiver [4], and $b = d + r$ for the passive receiver [5]. Also, α is the fraction of molecules that can be observed at the receiver from the time of their release until T, divided by the total number of molecules that would be observed at the receiver until infinite time. Meanwhile, the probability that a molecule released at $t = 0$ is observed by the receiver, reaches its global maximum at [5]

$$t_{\text{M}} = \frac{b^2}{6D}. \tag{2}$$

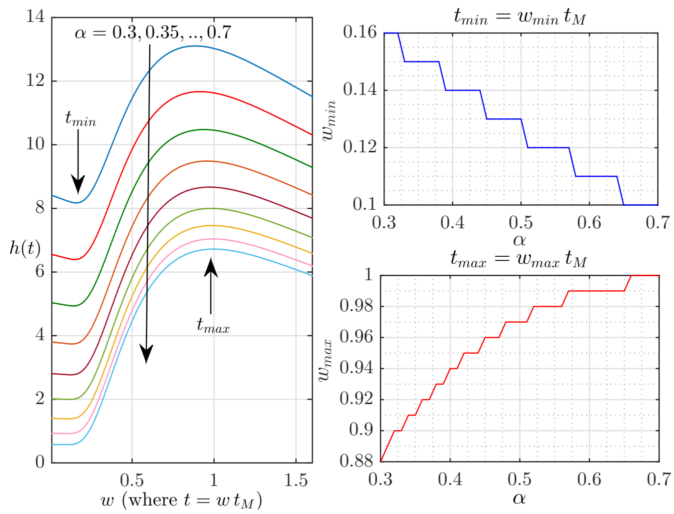

Fig. 2. $h(t)$, t_{min} and t_{max} for $I = 10$ and various values of α when the System 1 parameters of Table I (with $d = 5$ μm) are utilized.

III. Active Receiver

An active receiver absorbs the molecules that reach its surface and removes them from the communication environment. To this end, energy detection is employed, i.e., the receiver counts the molecules it absorbs within a predefined time interval. In [4], the first hitting probability function, corresponding to the probability that a single molecule transmitted at $t = 0$ is absorbed by the active receiver at time t, has been found to be

$$h(t) = \frac{r}{d+r}\frac{d}{\sqrt{4\pi D t^3}} \exp\left(-\frac{d^2}{4Dt}\right). \tag{3}$$

In the absence of ISI or in the case where α, and accordingly T, are high enough so that ISI is minimized, it is expected that the maximum number of molecules will be absorbed at t_{M}. However, this does not hold when the system suffers from typical ISI. In Fig. 2, $h(t)$ is depicted against $t = wt_M$. It can be easily observed that t_{min} equals the time when the ISI molecules become less than those corresponding to the current transmission. Moreover, the maximum number of molecules is received at t_{max}, which is lower than t_{M}, as can be seen in the bottom-right subfigure. As expected, t_{min} decreases and t_{max} increases with increasing α due to the decrease of ISI. It should be noted that the number of previously considered symbols, I, is set to 10 so as to guarantee that almost all the experienced ISI is taken into account.

As energy detection is based on the amount of absorbed molecules within a time interval, the expected fraction of molecules absorbed by the active receiver in $[t_1, t_2]$, with $t_1, t_2 \in [0, T]$ and $t_2 > t_1$, reads [4]

$$H_{\text{act}}(t_1, t_2) = \frac{r}{d+r}\left[\operatorname{erf}\left(\frac{d}{\sqrt{4Dt_1}}\right) - \operatorname{erf}\left(\frac{d}{\sqrt{4Dt_2}}\right)\right], \tag{4}$$

TABLE I
PARAMETERS OF THE MC SYSTEM

	System 1	System 2
D [m^2/sec]	10^{-9}	79.4×10^{-12}
d [μm]	$1, 2, 4, 5, 8, 10$	10
r [μm]	1	4

where $\text{erf}(\cdot)$ is the error function. If x_k and N_k^{act} are the kth transmitted bit and the number of received molecules corresponding to the kth transmission (or symbol) duration, respectively, then

$$N_k^{\text{act}} \sim \text{Pois}\left(\sum_{i=0}^{I} M x_{k-i} H_{\text{act}}(t_1 + iT, t_2 + iT) + \mu_N\right), \tag{5}$$

where μ_N is the mean value of the external noise molecules received in the same time interval and $Y \sim \text{Pois}(\lambda)$, implies that Y follows Poisson distribution with mean λ.

Utilizing the approximation of Poisson with a Gaussian distribution and an appropriate continuity correction [3], a closed-form expression for the mean error probability, P_e^{ED}, can be derived for the case of energy detection. If τ is the optimal threshold value that is computed numerically, then

$$P_e^{\text{ED}} = \left(\frac{1}{2}\right)^{I+2} \sum_{q=1}^{2^I} \left[\text{erfc}\left(\frac{\mu(q,1) - \tau + 0.5}{\sqrt{2\mu(q,1)}}\right) + \text{erfc}\left(\frac{\tau - 0.5 - \mu(q,0)}{\sqrt{2\mu(q,0)}}\right)\right], \tag{6}$$

where q corresponds to each of the 2^I possible bit sequences $\{v_1, v_2, .., v_I\}$ that stand for the I previous transmissions. Also, the mean value $\mu(q,x)$, where $x = \{0,1\}$ is the current bit value, reads

$$\mu(q,x) = M x H_{\text{act}}(t_1, t_2) + \sum_{j=1}^{I} [M v_j H_{\text{act}}(t_1 + jT, t_2 + jT)] + \mu_N. \tag{7}$$

In the existing literature, the utilized values of t_1 and t_2 are set equal to 0 and T, respectively, implying that the total number of observed molecules during a symbol duration is taken into account for the detection. In this paper, the aim is to show that utilizing different values for t_1 and t_2 results in lower error probability. Assuming $t_1 = w_1 t_M$, and given that the highest experienced ISI occurs at the beginning of the symbol interval, then selecting $t_1 > 0$ is expected to result in ISI mitigation. Furthermore, as $h(t)$ decreases significantly for $t > t_{\text{max}}$, it can be easily inferred that utilizing $t_2 = w_2 T$ where $t_2 < T$, may be advantageous. To this end, two systems with parameters given in Table I have been simulated, alongside with $M = 10^4$ and $I = 10$, unless otherwise stated.

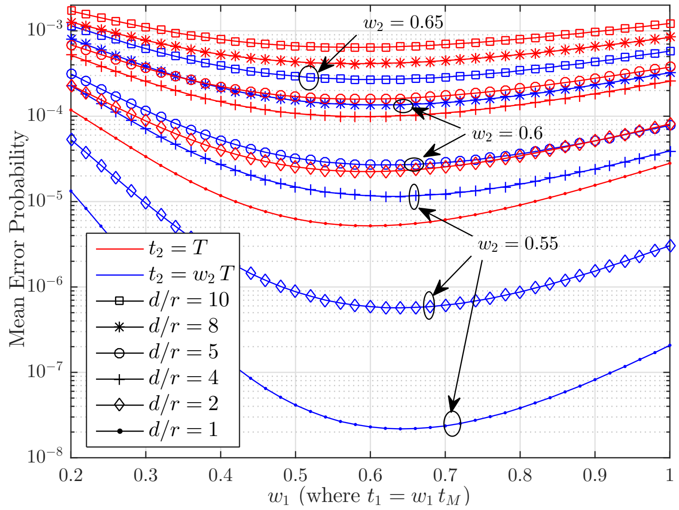

Fig. 3. P_e^{ED} versus w_1 for System 1 with $\alpha = 0.4$, where the optimal $t_2 = w_2 T$ value is plotted along with $t_2 = T$ for various d/r values.

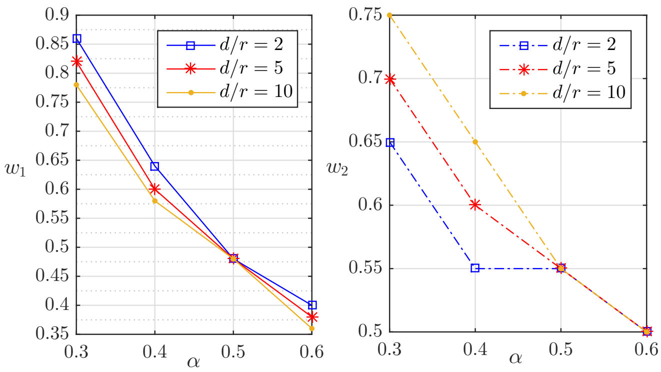

Fig. 4. Optimal values for w_1 and w_2 for various α and d/r.

Finally, the signal-to-noise ratio (SNR), γ_{ED}, is set equal to 10 dB, calculated by the formula

$$\gamma_{\text{ED}} = 20 \log_{10} \frac{0.5 M H_{\text{act}}(t_1, t_2)}{\mu_N}. \tag{8}$$

In Fig. 3, it is obvious that there exist optimal values of t_1 and t_2 that can tremendously enhance the error performance of the system by implementing energy detection. Furthermore, the increase in d/r results in increasing error probability, as expected, but at the same time results in higher w_2 and a slightly lower w_1. This increase of the time interval length $t_2 - t_1$ can be partly explained by the need to observe molecules for longer time due to the increase in the transmission distance. Interestingly, it has been observed that (4) can be written as

$$H_{\text{act}}(w_1, w_2) = \frac{1}{1 + (d/r)}\left[\text{erf}\left(\sqrt{\frac{3}{2w_1}}\right) - \text{erf}\left(\frac{[\text{erfc}^{-1}(\alpha)]^2}{\sqrt{w_2}}\right)\right], \tag{9}$$

which reveals that d/r and α are critical parameters for the optimal selection of w_1 and w_2 that enhance the system

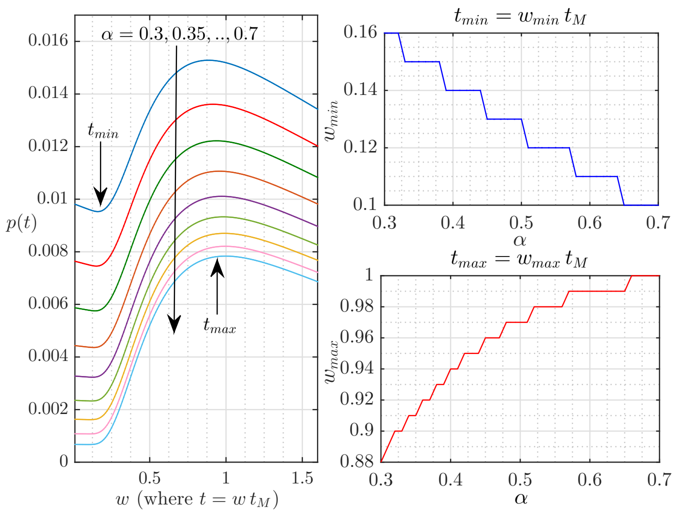

Fig. 5. $p(t)$, t_{min} and t_{max} for $I = 10$ and various values of α when the System 2 parameters of Table I are utilized.

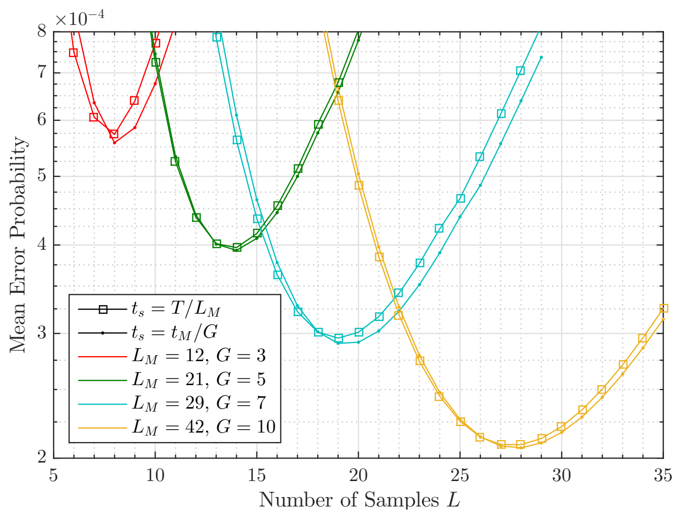

Fig. 6. P_e^{AD} versus L when $f(l) = lt_s$, $l = 1, 2, .., L$, and the System 2 parameters of Table I alongside with $\alpha = 0.4$ are utilized.

performance in terms of the error probability. To this end, the optimal values of w_1 and w_2 have been evaluated numerically and illustrated in Fig. 4 for several α and d/r.

IV. Passive Receiver

Passive receivers do not interact with the molecules that collide with their surface. As a result, a molecule may be observed more than once at the passive receiver. To this end, amplitude detection, where observations made at specific time instants and not during the whole time interval, is more commonly utilized as it has been proved more advantageous.

The probability that a single information molecule emitted at $t = 0$ lies within the passive receiver's volume, V, at t is [3]

$$p(t) = \frac{V}{(4\pi Dt)^{3/2}} \exp\left(-\frac{(d+r)^2}{4Dt}\right). \tag{10}$$

Interestingly, the behaviour of $p(t)$ depicted in Fig. 5 is analogous to that of $h(t)$ in Fig. 2. Also, w_{min} and w_{max} are equal to their corresponding values for the active receiver, because after substituting $t = wt_{\text{M}}$, we have

$$h(t), p(t) \propto \frac{1}{\sqrt{w^3}} \exp\left(-\frac{3}{2w}\right), \tag{11}$$

which implies that $h(t)$ and $p(t)$ differ only by a constant.

Assuming that L samples are taken by the receiver at time instants given by $f(l) \in [0, T]$, where $l = 1, 2, .., L$, and that they are summed up before the single threshold detection, then the number of received molecules corresponding to the lth sample taken within the kth transmission interval yields

$$N_{k,l}^{\text{AD}} \sim \text{Pois}\left(\sum_{i=0}^{I} M x_{k-i} p(f(l) + iT) + \mu_n\right), \tag{12}$$

where μ_n stands for the mean value of the noise molecules observed per time sample. Besides, the mean error probability for the amplitude detection, P_e^{AD}, reads

$$P_e^{\text{AD}} = \left(\frac{1}{2}\right)^{I+2} \sum_{q=1}^{2^I} \left[\text{erfc}\left(\frac{\sum_{l=1}^{L} \mu_l(q,1) - \tau + 0.5}{\sqrt{2\sum_{l=1}^{L} \mu_l(q,1)}}\right) + \text{erfc}\left(\frac{\tau - 0.5 - \sum_{l=1}^{L} \mu_l(q,0)}{\sqrt{2\sum_{l=1}^{L} \mu_l(q,0)}}\right)\right], \tag{13}$$

where the mean value $\mu_l(q, x)$ can be computed as

$$\mu_l(q, x) = Mxp(f(l)) + \sum_{j=1}^{I} [Mv_j p(f(l) + jT)] + \mu_n. \tag{14}$$

In most of the research works conducted so far [3], it has been assumed that the L samples taken within a time symbol duration correspond to time instants given by $f(l) = lt_s$, where $l = 1, 2, .., L$. Moreover, $t_s = T/L$ stands for the sampling time. Hereby, we aim to optimize a) the number of samples, L_{opt}, b) the time, t_1, when the first sample will be collected, c) the time, t_2, when the last sample will be collected, and d) the sampling time, t_s, while keeping the same time distance between all adjacent samples.

Motivated by the fact that the time where the maximum number of molecules is observed within the receiver, i.e., t_{max} is a fraction of t_{M}, a sampling time analogous to t_{M}, i.e., $t_s = t_{\text{M}}/G$ with $G \geq 1$, has also been considered. In the following, we have simulated a system with a passive receiver using the parameters of System 2 in Table I, $\alpha = 0.4$ and SNR, γ_{AD}, equal to 10 dB, which is calculated by the formula

$$\gamma_{\text{AD}} = 20 \log_{10} \frac{0.5M \sum_{l=1}^{L} p(f(l))}{L\mu_n}. \tag{15}$$

In Fig. 6, assuming that a maximum number of L_{M} samples can be taken in each case depending on the utilized sampling time, it is shown that using only the first L out of the L_{M} observations can be proven advantageous for the system

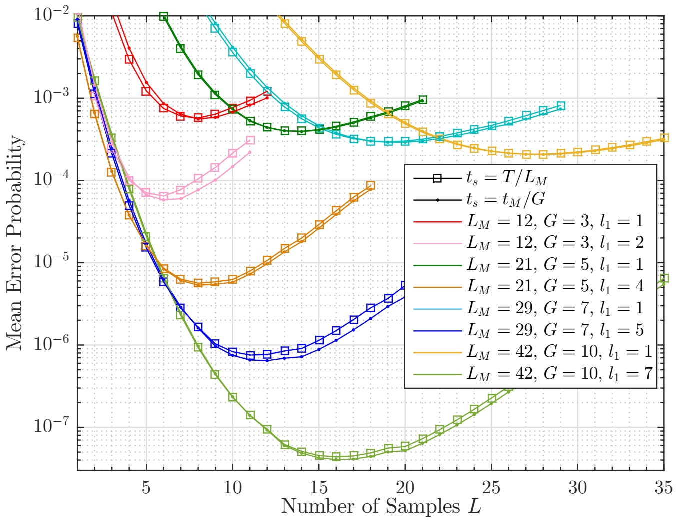

Fig. 7. P_e^{AD} versus L when $f(l) = (l_1 + l - 1)t_s$, where $l = 1, 2, .., L$ and System 2 parameters along with $\alpha = 0.4$ are utilized.

performance. For example, a system with $L_{\text{M}} = 29$ performs optimally in terms of error rate, when only the first $L_{\text{opt}} = 19$ samples are utilized. Besides, utilizing the sampling time t_{M}/G instead of T/L_m, causes the mean error probability in all illustrated scenarios to slightly decrease. We note that the maximum number of samples that can be collected when $t_s = t_{\text{M}}/G$ can be computed from

$$L_{\text{M}} = \left\lfloor \frac{T}{t_s} \right\rfloor = \left\lfloor \frac{3G}{2[\text{erfc}^{-1}(\alpha)]^2} \right\rfloor . \tag{16}$$

Finally, as a result of extensive simulations, it has been inferred that L_{opt} has a value close to

$$\left\lfloor L_{\text{M}} \frac{w_{\min} + w_{\max}}{2} \right\rfloor , \tag{17}$$

showing that the collection of samples should not continue until time T after the transmission but finish earlier.

Below, we indicate that the minimization of error probability can be further assisted by selecting the optimal time for the sampling process to begin. In Fig. 7, the observations are made at $f(l) = (l_1 + l - 1)t_s$, where $l = 1, 2, .., L$ and l_1 stands for the first sample that should be considered in the detection in order to achieve the minimum error probability. Thus, if $l_1 = 1$, the sampling begins at $t = t_s$, while if $l_1 \neq 1$, the sampling begins at $t = l_1 t_s$. Obviously, the value of l_1 that minimizes the mean error probability does not equal 1 and has been found equal to or slightly different than

$$\left\lfloor \frac{(w_{\min} + w_{\max})L_{\text{M}}}{3\,\text{erfc}^2(\alpha)} \right\rfloor + 1. \tag{18}$$

Thus, if L_{opt} is the number of samples that should be collected to minimize the probability of error, the last observation will be made at $t = (l_1 + L_{\text{opt}} - 1)t_s$. For instance, when $L_{\text{M}} = 42$ and $t_s = t_{\text{M}}/10$, we have that $l_1 = 7$ and $L_{\text{opt}} = 16$, thus the sampling will start at $7t_s$ and finish at $22t_s$.

Therefore, it was shown that, in the case of passive receiver, the optimization of the observations' timing results in significant enhancement of the error performance. Besides, the reduction in the number of samples that should be considered, decreases the receiver complexity, which is vital for MC. In this section, we have assumed that the collected samples are equally spaced in time. However, it would be interesting to examine whether the error performance can be further enhanced in the case where adjacent samples are not equally spaced in time. Although this is expected to increase the complexity and the requirements for synchronization at the receiver, its tangible effect will be considered in a future work.

V. Conclusion

Diffusion-based MC systems suffering from ISI and noise have been analysed in terms of the achievable error probability. It has been proved that optimizing the timing of the receiver's observations significantly enhances the error performance of the system. The optimal time interval for the observations to be made in the energy detection case has been evaluated numerically and found different from the commonly utilized $[0, T]$. Finally, regarding the amplitude detection, an improved sampling time has been proposed, while near optimal closed-form expressions for the number of samples and the first and the last sample that should be considered have been derived.

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