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Capacity analysis of a diffusion-based short-range molecular nano-communication channel

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ABSTRACT

Simulation-based and information theoretic models for a diffusion-based short-range molecular communication channel between a nano-transmitter and a nano-receiver are constructed to analyze information rates between channel inputs and outputs when the inputs are independent and identically distributed (i.i.d.). The total number of molecules available for information transfer is assumed to be limited. It is also assumed that there is a maximum tolerable delay bound for the overall information transfer. Information rates are computed via simulation-based methods for different time slot lengths and transmitter–receiver distances. The rates obtained from simulations are then compared to those computed using information theoretic channel models which provide upper bounds for information rates. The results indicate that a 4-input–2-output discrete channel model provides a very good approximation to the nano-communication channel, particularly when the time slot lengths are large and the distance between the transmitter and the receiver is small. It is shown through an extensive set of simulations that the information theoretic channel capacity with i.i.d. inputs can be achieved when an encoder adjusts the relative frequency of binary zeros to be higher (between 50% and 70% for the scenarios considered) than binary ones, where a 'zero' corresponds to not releasing and a 'one' corresponds to releasing a molecule from the transmitter.

1. Introduction

A nanonetwork is an interconnection of nanodevices which are made up of nanoscale components capable of performing simple computation, sensing, and actuation tasks [1]. Such an interconnection allows nanodevices to cooperate and share information. Nanonetworks will have significant applications in biomedicine, industrial process control, environmental pollution monitoring, and military surveillance. In nanonetworks, traditional silicon-based electromagnetic and acoustic communication technologies are not feasible due to their size, complexity and power requirement. So far, researchers have proposed two possible means by which nanodevices can communicate: molecular communication and nano-electromagnetic communication. Molecular communication [1–6] is proposed as a feasible alternative to traditional communication technologies at the nanoscale. In molecular communication, molecules are used to transmit messages (mainly, phenomena and chemical states) between nano-transmitters and nano-receivers. This offers a biocompatible and energy efficient means of information transmission both at short-range and at long-range, where short-range refers to distances from nanometers to millimeters and long-range refers to distances from millimeters to meters [1,5]. Nano-electromagnetic communication [7,8], on the other hand, is based on transmission and reception of electromagnetic radiation in the terahertz band using transceivers manufactured from novel nanomaterials such as graphene. Nano-electromagnetic communication is likely to be used for interconnecting nanosensors and nanoactuators in monitoring applications which may require high-speed information transfer. In general, nanonetworks may

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employ either or both modes of communication depending on the application at hand.

Diffusion-based short-range molecular communication is the basis of paracrine signaling in biological systems where the released molecules act on cells in the immediate vicinity (at distances of a few micrometers) of the transmitter [9]. For instance, in the nervous system, electrical signals travel long distances through the nerve cells called neurons, which in turn release neurotransmitters that diffuse a short distance to the target cell. Also, many signaling molecules that regulate development in multicellular organisms act at short range [9]. Diffusion-based communication has desirable properties: it is "rapid" over short distances and uses only the kinetic energy possessed by molecules without requiring input of energy from another source [9,10]. Molecular communication systems also involve the use of degrading enzymes that act on transmitted molecules and decompose them at an exponentially increasing rate. As such, the noise in the system will be due to random arrival times and degradation of diffusing molecules.

In this paper, diffusion simulations are conducted for a time-slotted molecular communication channel between a nano-transmitter and a nano-receiver to analyze information rates between channel inputs and outputs and to determine the information theoretic channel capacity when the inputs are independent and identically distributed (i.i.d.). The nano-transmitter and the nano-receiver are assumed to be synchronized with each other. This assumption, however, is not a restrictive one since there exist a number of nanodevice synchronization techniques [11] such as transmission of acoustic, optical or radio frequency synchronization pulses from an external source to nanodevices, or use of mobile nanodevices called "chronocytes" that are capable of synchronizing their neighbors to a universal time. Two discrete channel models are also used to approximate the channel and the information rates computed with these models are compared to those obtained via diffusion simulations. Capacity analysis of such channels is important for quantifying the maximum amount of information that can be transferred from a transmitter to a receiver with a given number of molecules and hence for assessing the practicality of this particular means of communication.

Recent work on the subject involves analysis of information rates that are possible with various propagation schemes (including diffusion) and miscellaneous noise reduction approaches [12]. However, the authors of the cited work assume equally likely binary input symbols and use empirical data from simulations to calculate the probability of successful communication and to account for communication errors due to channel memory when calculating information rates. Equally likely input symbols will generally yield lower channel capacity in non-symmetric channels. Further, the aforementioned paper attempts to characterize information rates of a unicast channel in bits per second for different time slot lengths and implicitly assumes that the length of the slots can be increased arbitrarily without violating a delay constraint. The conclusion that the information rate decreases with increasing slot length may thus be misleading since one should consider the total amount of time the channel will be used when calculating the information rate in bits per second [13,14]. In a closely related work [15], the capacity of a calcium relay channel is investigated using information theoretic methods and assumptions similar to those employed in [12]. In [16], the author derives bounds for the generally intractable information rates by employing tractable approximations for diffusion-based molecular communication channels. The paper gives some examples for computing information rates, but the assumptions on diffusion parameters are slightly impractical and derivation of good tractable approximations for practical systems is left as future work. In [17], the authors use inequalities and make certain distributional assumptions to analyze the capacity of channels where molecular concentrations are used to encode binary information. The channel model in [17], however, employs a transition matrix that does not comply with information theoretic definitions and may produce inaccurate results. Both [16,17] model the system as a simple discrete memoryless channel integrating the effect of late molecule arrivals (due to the uncertainty in diffusion) from previous intervals into the current transmission interval. Finally, in [18], a deterministic approach is taken to evaluate the capacities of point-to-point, broadcast, and multiple access molecular channels. Based on the derived deterministic models, the authors also analyze the information flow capacity of a diamond-like molecular nanonetwork.

The primary contribution of this work is the development of alternative and more elaborate simulation-based and information theoretic models for time-slotted diffusion-based short-range molecular nano-communication channels. As such, a simple discrete memoryless *Z*-channel model is first constructed to assess how well it can capture the behavior of a nano-communication channel. In diffusion-based molecular communication systems, however, channels have "memory" which is due to still-diffusing molecules from previous transmission intervals. Therefore, a discrete memoryless channel model with an extended input alphabet is then constructed to represent a channel with one-stage memory. Simulation- and model-based results are analyzed and compared to give quantitative insights into design of nano-communication systems.

The rest of the paper is organized as follows: In Section 2, a diffusion simulation model for the nano-communication channel is developed. Information theoretic channel models that will provide upper bounds for information rates are also described in the same section. Information rates obtained via simulations and by using the channel models are presented in Section 3. Section 4 concludes the paper.

2. Methods

Two types of encoding techniques have been identified for nanonetworks that employ molecular communication [1,3]: information can be encoded by varying the temporal concentration of specific molecules in the medium, or it can be encoded directly on the molecule itself. Here, a simple "on–off signaling" technique also used in [12] is con-

sidered where the emission of a single molecule corresponds to an "on" signal. Hence, it will be assumed that binary information is encoded as follows: release of a single molecule from the transmitter corresponds to a '1', and no release corresponds to a '0' during a channel use or a transmission interval. The time will be divided into T-millisecond-long transmission intervals, which are called slots, and the communication is successful if the transmitter and the receiver agree on what is sent during T over the aqueous channel. Encoding a '1' onto only one molecule requires a high degree of sensitivity of the receiver so that a single molecule is sufficient for detecting the signal. In practice, it is also possible to send multiple molecules and require reception of a given number of molecules per time slot to increase the probability of communicating a '1' and to reduce the receiver's sensitivity to noise [12].

In traditional communication systems, transmission is subject to a power constraint and takes place over bandwidth limited channels. For the molecular communication systems considered here, on the other hand, the following constraints are in effect: there are a given number of molecules available for communication and the maximum tolerable total delay for transmitting the overall information is bounded. The first constraint is due to the fact that synthesizing molecules within a nanodevice can be prohibitive so that a nano-transmitter usually has a finite reservoir of molecules which are obtained externally [1,16]. The constraint of having a given number of molecules implies limiting the total number of channel uses or time slots for transferring information. Imposing a bound on the overall delay is a corollary of the fact that arbitrarily long waits for the information transfer are unacceptable for many systems since late information is useless for many applications.

2.1. Information rate and capacity

The mutual information rate (or simply, the information rate) [13] between the input and the output of the channel is given by

$$R = \lim_{N\to\infty} \frac{1}{N} I(X^N; Y^N) = \lim_{N\to\infty} \frac{1}{N} I(X_1, \ldots, X_N; Y_1, \ldots, Y_N), \quad (1)$$

where $I(\cdot;\cdot)$ denotes the mutual information, $X^N = (X_1, \ldots, X_N)$ is the binary input process of the channel, and $Y^N = (Y_1, \ldots, Y_N)$ is the binary output process of the channel. If Q is the distribution of the input sequence, the channel capacity is given by

$$C = \lim_{N\to\infty} \max_{Q} \frac{1}{N} I(X^N; Y^N). \quad (2)$$

For the present work, it will be assumed that the channel inputs are i.i.d. with a common distribution $Q(x) = \mathbb{P}(X = x)$ where $x \in \{0,1\}$ and $Q(0) = \alpha$ for $0 \leqslant \alpha \leqslant 1$. The i.i.d.-input capacity of the channel is then calculated by maximizing the information rate over α.

In general, calculation of the information rate is a hard problem when each sample of the output process depends statistically both on the corresponding input and on past inputs. Such a situation arises very frequently in communication theory when studying channels with memory. Molecular communication channels considered here have memory which is due to still-diffusing molecules from previous transmission intervals. Despite the complexity of the problem, in many practical signal analysis applications, one can treat the input and output processes of the channel as two time series and employ the well-studied tools and techniques for estimation of mutual information between two time series (see, for example, [19] and the references therein). To this end, binary input and output samples generated by simulations will be treated as time series. Let X and Y denote the discrete random variables representing the observations of the channel input and output processes at steady-state, respectively. The well-known mutual information formula between X and Y [13] is used to calculate an estimate $\widehat{R}$ of the information rate:

$$\widehat{R} = I(X;Y) = \sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x,y) \log_2 \left(\frac{p(x,y)}{p(x)p(y)} \right), \quad (3)$$

where $\mathcal{X}$ and $\mathcal{Y}$ denote the input alphabet and the output alphabet, respectively. The estimate can be obtained by "plugging in" the empirical probabilities corresponding to marginal probabilities, $p(x) = \mathbb{P}(X = x) = Q(x)$ and $p(y) = \mathbb{P}(Y = y)$, and joint probabilities $p(x,y) = \mathbb{P}(X = x, Y = y)$ for the discrete random variables X and Y.[1] In this work, `mi 0.9` software toolbox [21] is used to calculate information rates between binary input and output sequences generated by simulations.

The information rates and capacities are reported in units of *bits per channel use*. For systems with equal overall delay bound, a channel with more capacity in terms of bits per channel use will transfer more information in a given number of time slots. In this work, diffusion simulations are carried out for $N = 10{,}000$ time slots over the range of values of α. This choice of N proves sufficient since the standard errors associated with the estimates reported in Section 3 are within 5% of the averages computed over five simulations, establishing the convergence of simulation results.

2.2. Molecular movement as a diffusion process

In the systems considered, the molecules released from the transmitter move to a close-proximity receiver via passive diffusion. When the distance d between a point-transmitter and a receiver is small compared to the radius of the receiver, the receiver can be modeled as a plane. The receiver is assumed to have a sufficient density of molecular receptors and can instantaneously intercept molecules whenever they hit its surface. With these assumptions, the movement of molecules can be modeled as a one-dimensional Wiener process [22]. Similar modeling assumptions were also made in [16]. Fig. 1 shows the configuration of the transmitter and the receiver that will be used throughout the paper. According to the Wiener model, if the receiver is at a distance d, the first-hitting time

[1] The empirical probability [20] is obtained by dividing the number of occurrences of an event by the number of observations. If the number of observations is large, the empirical probability converges to the true probability with probability 1.

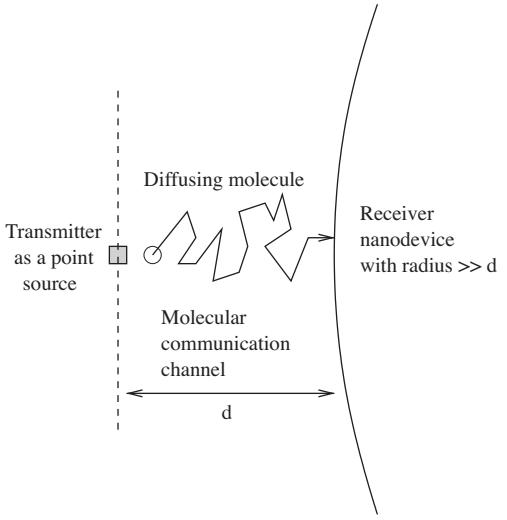

Fig. 1. A diffusion-based short-range molecular communication channel. The molecules are emitted from a transmitter that is modeled as a point source. The radius of the receiver is assumed to be much larger than the distance between the transmitter and the receiver.

probability density for a single released molecule is given by

$$f(t) = \frac{|d|}{(2\pi\sigma^2 t^3)^{1/2}} \exp\left(\frac{-d^2}{2\sigma^2 t}\right), \quad t \geqslant 0, \tag{4}$$

with $\sigma^2 = 2D$, where D is the diffusion coefficient. For small molecules, $D \sim 10^{-9}\,\mathrm{m}^2/\mathrm{s}$ in water at 310 K, whereas for large molecules, $D \sim 10^{-11}\,\mathrm{m}^2/\mathrm{s}$ [11]. In this work, it will be assumed that a '1' is transported by a small molecule. If large molecules were used as transporters, the information rates achieved would be smaller for given T and d.

2.3. Stochastic degradation of molecules in simulations

Molecular communication systems often involve the use of degrading enzymes so that diffusing molecules are decomposed or deactivated in time [3,5,12]. Degraded molecules with their altered structures are no longer recognized as valid signals and cannot bind to a receiver's receptors. Such a degradation mechanism is introduced to reduce possible interference to communication in future time slots. In order to have a realistic assessment of system performance, the diffusion simulations account for stochastic degradations. Molecules are assumed to have lifetimes that follow a Weibull(a,b) distribution [20] which can be used to model lifetimes with an increasing failure rate when the shape parameter b is greater than 1 (i.e., the molecules experience "ageing"). The scale parameter $a > 0$, on the other hand, is a measure of the spread of the distribution. A positive random variable is said to be Weibull(a,b) distributed if it has the density [20]

$$w(x) = \frac{b}{a}\left(\frac{x}{a}\right)^{b-1} \exp\left[-\left(\frac{x}{a}\right)^{b}\right], \quad x \geqslant 0. \tag{5}$$

The mean of the Weibull(a,b) distribution is $\tau = a\Gamma(1 + 1/b)$, where $\Gamma(\cdot)$ is the Gamma function [20]. A molecule is eliminated from the system when it reaches the receiver or when its lifetime expires.

2.4. Approximations with discrete memoryless channel models

Two information theoretic models that approximate the nano-communication channel will be used to analyze the information rates. The input alphabet and the output alphabet are denoted by $\mathcal{X}$ and $\mathcal{Y}$, respectively. Both models are constructed to obtain simple but insightful approximations and are used to provide upper bounds for information rates. In these models, it will be assumed that the lifetimes of molecules are deterministic.

2.4.1. The Z-Channel

If one assumes an idealized system in which there is no stochastic degradation of molecules and the molecules are eliminated at the end of the time slot, the channel errors are only due to the released molecules not arriving by the end of a transmission slot. As such, the channel can be modeled as a discrete memoryless Z-channel [13,14] with $\mathcal{X} = \mathcal{Y} = \{0,1\}$ as illustrated in Fig. 2. The channel transition matrix $\mathbf{P}(y|x)$ is defined as follows. The entry in the xth row and yth column is the conditional probability $p(y|x)$ that y is received when x is transmitted:

$$\mathbf{P}(y|x) = \begin{bmatrix} 1 & 0 \\ 1-r & r \end{bmatrix} \tag{6}$$

with

$$r = \int_0^T f(t)dt \tag{7}$$

denoting the probability of a single released molecule successfully hitting the receiver during a transmission slot, where $f(t)$ is given by Eq. (4). The input distribution for this channel model is specified by

$$Q(0) = \mathbb{P}(X = 0) = \alpha, \quad \text{and} \quad Q(1) = \mathbb{P}(X = 1) = (1 - \alpha). \tag{8}$$

2.4.2. A 4-input–2-output discrete memoryless channel

If another idealized system is considered where there is no stochastic degradation of molecules and the molecules are eliminated at the end of two time slots after their release, one has to take into account possible interference that may be caused by "late" molecules from the previous time slot, and the Z-channel model can be extended as follows. First, the probability s of a single released molecule hitting the receiver during its own transmission slot when the previous input was a '0' and the probability n of receiving a '1' from the previous slot when no molecule is re-

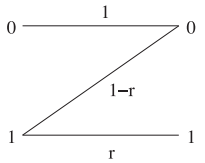

Fig. 2. The discrete memoryless Z-channel model for approximating the diffusion-based short-range molecular communication channel.

leased in the current transmission slot are defined using the first-hitting time probability density given in Eq. (4) as:

$$s = \int_0^T f(t)dt, \tag{9}$$

and

$$n = \int_T^{2T} f(t)dt. \tag{10}$$

Then, a discrete memoryless channel model is constructed as illustrated in Fig. 3. In this model, the input alphabet is extended to four symbols $\mathcal{X} = \{00, 01, 10, 11\}$ to account for interference from (or the channel memory due to) "late" molecules from the previous slot. Each input symbol consists of two bits: the leftmost bit corresponds to communication during the previous slot and the rightmost bit corresponds to the current communication. The output alphabet is again $\mathcal{Y} = \{0, 1\}$. Accordingly, the channel transition matrix $\mathbf{P}(y|x)$ is defined as follows:

$$\mathbf{P}(y|x) = \begin{bmatrix} 1 & 0 \\ 1-s & s \\ 1-n & n \\ (1-n)(1-s) & 1-(1-n)(1-s) \end{bmatrix}. \tag{11}$$

The input distribution for this channel model is constrained by

$$Q(00) = \mathbb{P}(X = 00) = \alpha^2, \quad Q(01) = \mathbb{P}(X = 01) = \alpha(1-\alpha),$$
$$Q(10) = \mathbb{P}(X = 10) = (1-\alpha)\alpha, \quad Q(11) = \mathbb{P}(X = 11) = (1-\alpha)^2. \tag{12}$$

We can refer to the channel with four possible inputs and two possible outputs as a 4-input–2-output channel.

2.4.3. Calculation of mutual information

Rewriting Eq. (3) to highlight its dependence on channel transition probabilities $p(y|x)$, we can calculate the mutual information of a discrete memoryless channel with input X and output Y as [13]

$$I(X;Y) = \sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} Q(x)p(y|x)\log_2\left(\frac{p(y|x)}{\sum_{x'\in\mathcal{X}} Q(x')p(y|x')}\right). \tag{13}$$

All the necessary quantities that appear in Eq. (13) are computed using Eqs. (6)–(8) for the Z-channel or Eqs. (9)–(12) for the 4-input–2-output discrete memoryless channel. The maximum information rates of discrete memoryless channels with specified input distributions can be calculated by maximizing Eq. (13) over α.

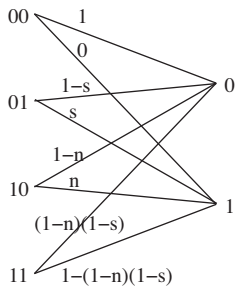

Fig. 3. A 4-input–2-output discrete memoryless channel model for approximating the diffusion-based short-range molecular communication channel.

3. Results

3.1. Exploratory analysis

First, an exploratory analysis was conducted to assess the effects of the choice of time slot length T and mean lifetime τ of molecules on information rates. Since the overall delay bound is given by NT, different values of T correspond to different maximum overall delay bounds acceptable by the system using the information. Transmitter–receiver separations used in the analysis were $d = 1$ and 2 μm. This length scale was compatible with paracrine signaling that has a range of a few micrometers and was also consistent with the separation distances investigated for diffusion-based molecular communication in previous work [12]. The chosen separation distances also justify the assumption made in Section 2.2 where molecular movement is modeled as a one-dimensional Wiener process; the separation distance is at least an order of magnitude less than the size of the envisioned bio-inspired nanodevices [1] typically having the size of a biological cell (10–100 μm [9]). The time slot lengths and mean lifetimes considered were $T = 1$, 10, 100 ms and $\tau = 1$, 10, 100 ms. The choice of the millisecond time scale for slot lengths was based on the fact that a small molecule with $D \sim 10^{-9}$ m^2/s moves away a distance of one or more micrometers in one millisecond with 50% probability [10]. One millisecond is also taken as a rough estimate of diffusion time for small particles over a micrometer [10]. The mean lifetime parameter was assumed to be adjustable either through the use of different types of molecules or through varying the concentration of degrading enzymes in the environment. For each molecule, a hitting time was generated based on Eq. (4) and a lifetime was assigned based on a Weibull $(\tau/\Gamma(1.5), 2)$ distribution.

Maximum information rate estimates (over α) in bits per channel use obtained for $d = 1$ and 2 μm are tabulated in Tables 1 and 2. Each reported value was obtained by averaging the results of five independent diffusion simulation runs. The standard errors associated with the estimates are also included in the tables. The results indicate that for a given time slot length T, the maximum information rate is the highest when the mean lifetime is "matched" to T. Hence, in this work, the lifetimes of molecules are assumed to follow a Weibull$(T/\Gamma(1.5), 2)$ distribution. Based on this model, the probability that a molecule

Table 1
Maximum information rate in bits per channel use when transmitter–receiver separation distance is $d = 1$ μm.

	$\tau = 1$ ms	$\tau = 10$ ms	$\tau = 100$ ms
$T = 1$ ms	0.2133 ± 0.0028	0.1541 ± 0.0034	0.1358 ± 0.0027
$T = 10$ ms	0.2743 ± 0.0011	0.5751 ± 0.0040	0.5171 ± 0.0053
$T = 100$ ms	0.2750 ± 0.0021	0.6124 ± 0.0062	0.8089 ± 0.0037

Table 2
Maximum information rate in bits per channel use when transmitter–receiver separation distance is $d = 2$ μm.

	$\tau = 1$ ms	$\tau = 10$ ms	$\tau = 100$ ms
$T = 1$ ms	0.0416 ± 0.0020	0.0187 ± 0.0009	0.0148 ± 0.0004
$T = 10$ ms	0.0810 ± 0.0012	0.3728 ± 0.0026	0.3030 ± 0.0052
$T = 100$ ms	0.0813 ± 0.0009	0.4144 ± 0.0016	0.6904 ± 0.0051

survives for a time period greater than T ms is 46% and the probability that a molecule survives for a time period greater than $2T$ ms is 4%. To this end, using one-stage memory when modeling the nano-communication channel may thus be appropriate.

One has to note that if the communication *were* tolerant to delay, the time slot length could be increased to achieve higher capacities for a given mean lifetime τ, as demonstrated by the results in Tables 1 and 2. However, the values for $\tau = 1$ ms indicate that even though an order of magnitude increase in the slot length relative to the mean lifetime leads to an improvement in capacity, more than an order of magnitude increase does not appear to result in any further benefit.

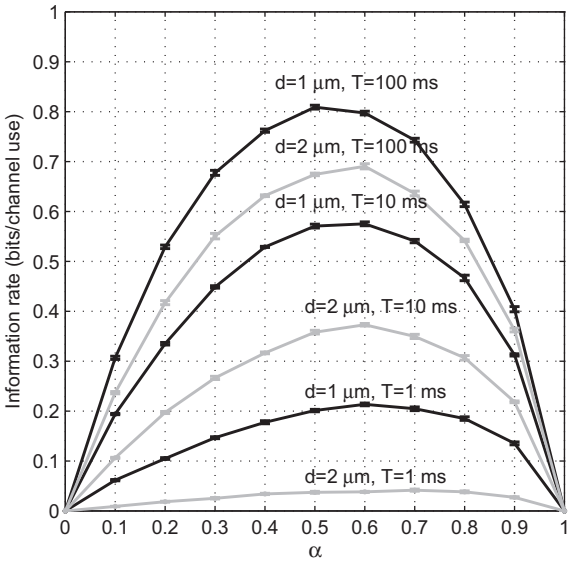

Fig. 4. Information rate in bits per channel use for different values of d and T. The values correspond to the results averaged over five diffusion simulations.

3.2. Simulation-based capacity analysis

The results of diffusion simulations for $T = 1, 10, 100$ ms (with corresponding "matched" mean molecule lifetimes $\tau = 1,\ 10,\ 100$ ms) and transmitter–receiver separations $d = 1$ and 2 μm are shown in Fig. 4. Information rate estimates for different values of α averaged over five simulations are plotted with the corresponding standard error bars. The standard errors were very small with the maximum standard error associated with the reported values being 0.0055 bits. The information rates in bits per channel use were higher when the transmitter–receiver distance was smaller for a given slot length. This conclusion is substantiated by the fact that diffusion is "rapid" over short distances but much slower over long distances. Therefore, successful communication is more likely when a molecule gets a chance to reach its destination before the next time slot. A key observation is that the concave information rate curves are not symmetric about $\alpha = 0.5$ (equally likely input) and this asymmetry is more pronounced for small T and large d. To be more precise, the maximum of information rate is attained when $\alpha > 0.5$.

For a more detailed analysis of parameter dependence, diffusion simulations were carried out to compute the information rate for a range of T when $d = 1$ μm and for a range of d when $T = 10$ ms. The results averaged over five

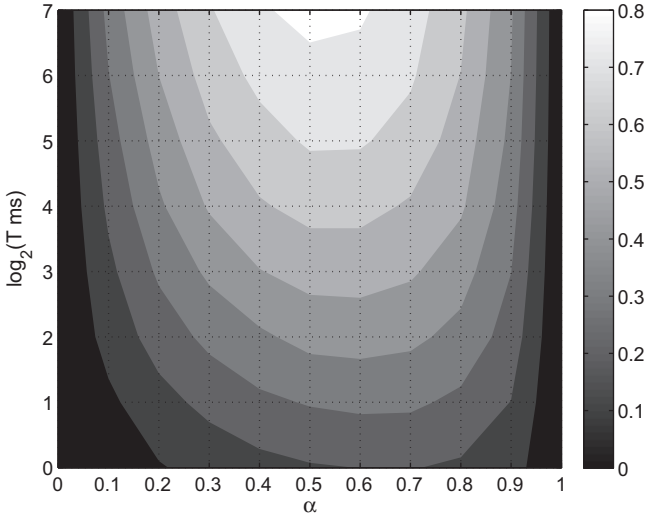

Fig. 5. Information rate in bits per channel use for different T when $d = 1$ μm.

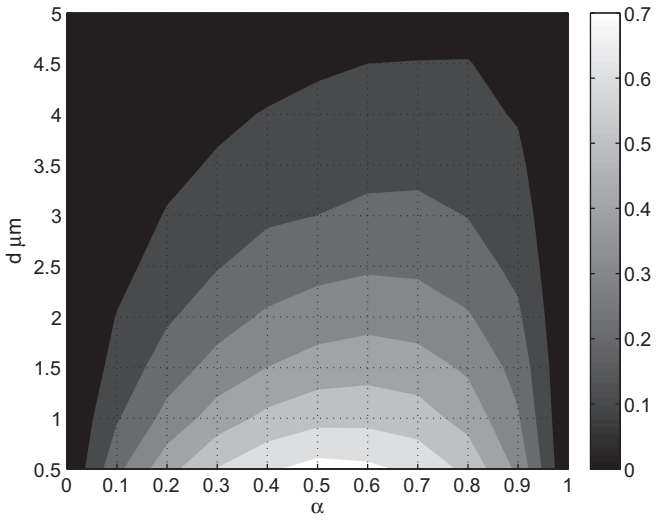

Fig. 6. Information rate in bits per channel use for different d when $T = 10$ ms.

simulations are plotted in Figs. 5 and 6. The contour plots in Fig. 5 show that the information rate curves are asymmetric about $\alpha = 0.5$ for systems with short time slot lengths. From Fig. 6, it can be seen that the information rate increases as the transmitter–receiver distance decreases for a given α. Also, the asymmetry of the curves increases as d gets larger. The i.i.d.-input channel capacity, which is defined as the maximum information rate over α, is generally achieved when not releasing a molecule is more probable than releasing one (i.e., $\alpha > 0.5$). That is, an encoder should adjust the relative frequency of binary zeros to be higher than binary ones ($0.5 \leqslant \alpha \leqslant 0.7$ for the scenarios considered). The channel capacity in bits per channel use is achieved with equally likely binary input symbols (i.e., when $\alpha = 0.5$ as was the assumption in [12]) when the time slot length is large (see Fig. 5) or when the transmitter–receiver distance is small (see Fig. 6).

3.3. Comparison of simulation results with approximate channel models

Recall that in Section 2.4, idealized systems were considered in which there was no stochastic degradation of molecules, and the released molecules were eliminated at the end of one time slot in the case of the Z-channel, or at the end of two time slots in the case of a 4-input–2-output channel. In other words, molecules had deterministic lifetimes. The validity of these assumptions can be investigated by comparing the results obtained using the models with the results from simulations. The information rates computed using the models described in Sections 2.4.1 and 2.4.2 are plotted in Figs. 7 and 8 together with the results obtained from simulations. The solid lines correspond to values obtained from diffusion simulations whereas the dashed lines correspond to values calculated using the channel models. The dashed curves in the figures represent upper bounds on the information rates since the noise due

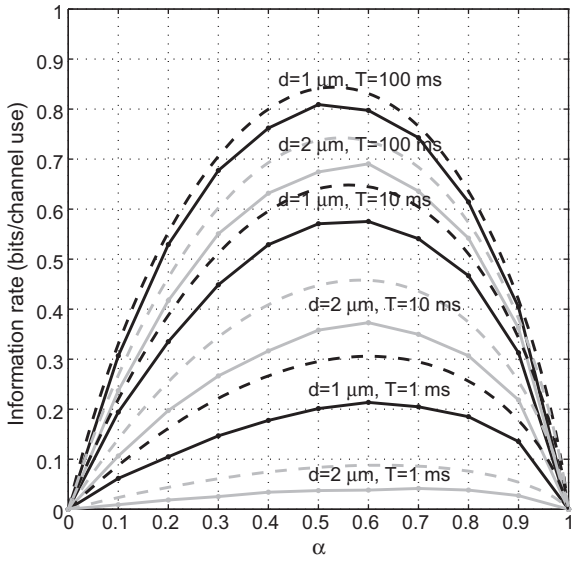

Fig. 7. Comparison of simulation and model-based information rates in bits per channel use for different values of d and T. The solid lines correspond to values obtained from diffusion simulations whereas the dashed lines correspond to values calculated using the Z-channel model.

to stochastic degradation of molecules is ignored in the idealized information theoretic models. Table 3 reports the sum of squared pointwise differences of 11 values obtained for different α and plotted in Figs. 7 and 8. The diffusion simulation results are in better agreement with the 4-input–2-output discrete memoryless channel (DMC) model. It can be claimed that the 4-input–2-output model well captures the channel's one-stage memory characteristic. The only case where the Z-channel provides a better approximation for the diffusion simulation results is when $T = 1$ ms and $d = 2$ μm. This is mainly due to compensation of late molecules by ones from the previous time slots in

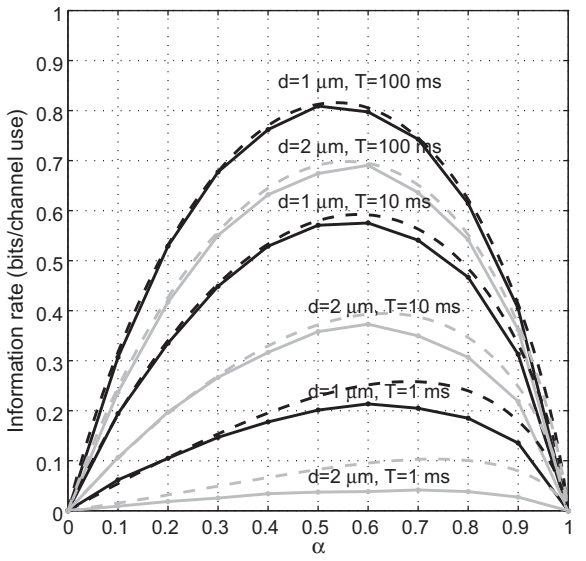

Fig. 8. Comparison of simulation and model-based information rates in bits per channel use for different values of d and T. The solid lines correspond to values obtained from diffusion simulations whereas the dashed lines correspond to values calculated using a 4-input–2-output discrete memoryless channel model.

Table 3
Sum of squared pointwise differences for assessing how well the information theoretic models approximate the nano-communication channel.

Configuration		Z-channel	4-Input-2–output DMC
T = 1 ms,	d = 1 μm	0.0498	0.0105
T = 10 ms,	d = 1 μm	0.0286	0.0017
T = 100 ms,	d = 1 μm	0.0068	0.0004
T = 1 ms,	d = 2 μm	0.0125	0.0175
T = 10 ms,	d = 2 μm	0.0475	0.0047
T = 100 ms,	d = 2 μm	0.0191	0.0011

the 4-input–2-output channel model which results in higher information rates. Such compensation may not occur in diffusion simulations wherein stochastic degradations are in effect. The compensation effect is particularly pronounced in the high α regime.

4. Conclusion

Nanonetworks have significant potential applications in a wide range of areas. However, the researchers have only recently started to analyze the performance of such networks. Molecular communication is expected to be one of the primary modes of communication between two nanodevices. In this paper, simulation-based and information theoretic models for a diffusion-based molecular nano-communication channel are presented. The developed models build on previous work in the field but provide more elaborate and precise methods for analyzing such channels. Analysis of information rates is expected to provide a useful insight into the capacity of such nano-communication channels and guide the design of nanonetworks that employ diffusion-based short-range molecular communication. In particular, the findings may prove useful in encoder design for molecular communication systems. However, the characterization and analysis of nano-communication channels are far from complete. Future work on the subject may involve creation of test beds and sophisticated simulation frameworks tailored for designing and testing signal processing components of nano-communication transceivers.

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