Rate-Delay Tradeoff With Network Coding in Molecular Nanonetworks

Bige D. Unluturk, *Student Member, IEEE*, Derya Malak, *Student Member, IEEE*, and Ozgur B. Akan, *Senior Member, IEEE*

***Abstract*—Molecular communication is a novel nanoscale communication paradigm, in which information is encoded in messenger molecules for transmission and reception. However, molecular communication is unreliable and has highly varying long propagation delays mainly due to the stochastic behavior of the freely diffusing molecules. Thus, it is essential to analyze its delay characteristics, as well as the tradeoff between the rate and delay, in order to reveal the capabilities and limitations of molecular information transmission in nanonetworks. In this paper, first, a new messenger-based molecular communication model, which includes a nanotransmitter sending information to a nanoreceiver, is introduced. The information is encoded on a polyethylene molecule, $CH_3(CHX)_nCH_2F$, where X stands for H and F atoms representing 0 and 1 bits, respectively. The emission of the molecules is modeled by puffing process which is inspired by the alarm pheromone release by animals in dangerous situations. In this work, the rate-delay characteristics of this messenger-based molecular communication model are explored. Then, a Nano-Relay is inserted in the model, which XOR's the incoming messages from two different nanomachines. Performance evaluation shows that indeed, a simple network coding mechanism significantly improves the rate given delay of the system, and vice versa.**

***Index Terms*—Molecular communication, molecule puffing, nanonetwork coding, rate-delay tradeoff.**

I. Introduction

ADVANCES in nano- and bio-technology require the development of biocompatible nanomachines, which have fundamental roles in complex biohybrid structures. These machines have a wide range of duties such as assisting the biological cells in performing the sustainment of vital activities and taking charge of disorders in biological entities, i.e., molecules, cells, and organs. In order to attain macroscale objectives, nanomachines need to communicate with each other to realize cooperative tasks, which leads to the development of nanoscale communication techniques. Molecular communication, as one of these techniques, is inspired by the natural behaviors of the existing biological structures, which paves the way for upcoming communication applications in nanoscale environments.

Since molecular communication inherently exists in nature, it is biocompatible, biostable and it has also the capability of operating at nanoscale. Hence, it may be applied to a wide variety of areas such as environmental applications, which include water and air pollution control, industrial applications, which include development of nanorobots, nanoprocessors and nanomemory, and medical applications, which are drug delivery, disease treatment, and health monitoring [1].

Despite the novelty of molecular commmunication, there are several physical implementations such as [3] where Cu^{2+} ions are used as information carrying molecules. With the help of fluorescence microscopic observations, in [4], the hybridization of DNA is used to employ a molecular communication path between vesicles. A physical reception mechanism is discussed in [5], where a biomimetic nanosensory device is implemented for detection and amplification of biologically important entities.

In the literature, the studies are concentrated on modeling [6], capacity [7], [8], noise analysis of molecular channels [9], and gain and delay with respect to input frequency and transmission range [6]. None of these studies investigates the rate-delay tradeoff in molecular domain, which is very crucial to determine the possible application areas. One of these areas is delay tolerant networks used for applications such as health monitoring, drug delivery, and molecular computers [1], [15].

Molecular communication differentiates from standard wireless communications with its dramatically higher and varying propagation delays [2], even up to hours [11], its operational uncertainties and proneness to noise and interference, due to diffusion of large molecules. Moreover, the nanomachine spends time generating multiple redundant molecules for a single message to guarantee the delivery of the message and preparing them for transmission. This unfortunately yields low rates. Therefore, a joint rate and delay analysis for molecular communication is needed to investigate its capabilities and shortcomings.

In classical communications domain, the rate-delay tradeoffs are examined to accommodate different types of traffic in electromagnetic networks with composite links [16], to optimize rate for two-layered, namely, physical and network packet transmission system [17], and mitigate delay in multipath routed and network coded networks [18]. Albeit these studies point out the rate-delay tradeoffs for classical communication domains, no study has concentrated on the tradeoff between rate and delay in molecular communications, which led us to this very study.

Manuscript received December 9, 2011; revised October 9, 2012; accepted December 3, 2012. Date of current version March 6, 2013. This work was supported in part by the Turkish Scientific and Technical Research Council Career Award under Grant #109E257, in part by the Turkish National Academy of Sciences Distinguished Young Scientist Award Program, and in part by IBM through IBM Faculty Award. The review of this paper was arranged by Associate Editor C. A. Moritz.

The authors are with the Next-Generation and Wireless Communications Laboratory, Department of Electrical and Electronics Engineering, Koc University, Istanbul 34450, Turkey (e-mail: bunluturk@ku.edu.tr; dmalak@ku.edu.tr; akan@ku.edu.tr).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/TNANO.2013.2241449

In this paper, a new diffusion-based model for molecular communication, whose main distinction with respect to previously proposed models, such as [6] and [7], arises from the utilization of a messenger molecule as information carrier, is introduced. A hydrofluorocarbon molecule, fluorinated polyethylene, is chosen as the messenger molecule on the grounds of biocompatibility of hydrofluorocarbons, which are the basic molecules used as reversible oxygen carriers in artificial blood formulations [19].

We analyze the stochastic nature of a basic point-to-point messenger-based molecular communication model with one nanotransmitter and one nanoreceiver, named Nano-Alice and Nano-Bob, respectively. Furthermore, a nanonetwork consisting of two nanomachines and a Nano-Relay is established. Then, a simple network coding is applied on this nanonetwork, and the rate and delay for both uncoded and network coded cases are derived to reveal the tradeoff between propagation delay and reception rate. With network coding, we attain higher rates with the same delay compared to the uncoded case, and lower delays for the same rate of operation, as discussed in Section IV.

The remainder of this paper is organized as follows. Using the messenger-based molecular communication model introduced in Section II, we investigate the delay characteristics of this model. In Section III, to examine an analysis of rate-delay tradeoff over a networking case with a single Nano-Relay, a simple network coding is applied. The expressions derived in Section II and III are evaluated numerically and the results on the rate-delay tradeoff are discussed thoroughly in Section IV. Finally, in Section V, a brief conclusion is given.

II. Messenger-Based Molecular Communication Model

Messenger-based molecular communication inherently exists in different types of cells from the simplest prokaryotic cells such as bacteria using quorum sensing to more complex mammalian cells using intracellular communication [20]. For example, nitric oxide, an intracellular messenger molecule, provides cell-to-cell communication in mammalians, which is exploited in artificial intracellular communication for gene regulation [20]. Since messenger-based molecular communication is ubiquitous, it is crucial to model it by benefiting from inherent communication mechanisms, which also promotes nanomedicine applications.

In this paper, a messenger-based molecular communication model is proposed. This model includes partially fluorinated polyethylene messenger molecules, $\mathrm{CH_3(CHX)_nCH_2F}$, carrying n bits of information on predefined X atoms by diffusion. X is replaced by an hydrogen (H) or fluorine (F) atom representing the bit 0 or 1. n can reach up to 10^9 bits, which is a practically high amount of information for a single molecule despite its longer propagation delay [11]. Therefore, the messenger-based approach is an intriguing case for realizing the rate-delay tradeoff.

In our model, the transmitter nanomachine is capable of producing molecules on which the information is encoded, combining them into puffs, and releasing the puffs to the medium where they are propagated by Brownian motion with drift which arises from the mean drift velocity of the fluid medium. The receiver nanomachine, which has the receptors that bind the propagating molecules, is capable of picking the molecules, and decoding them. The radii of these nanomachines are assumed to be a few nanometers. Hence, they are capable of handling fluorinated polyethylene molecules, the size of which is $10^{-2} \times n$ nm^3. Moreover, they are assumed to be separated by a few micrometers so that the size of the nanomachines are negligible compared to the distance traveled by the messenger molecule [11].

Our model embodies five main processes; information encoding process, transmission process, propagation process, reception process, and information decoding process. In the following sections, we investigate these five main processes.

A. Information Encoding Process

In this model, it is assumed that nanomachines use information-storing packets, i.e., messenger molecules for the transfer of information which are similar to data link-layer packets in classical wireless communication systems. These two differ in that the molecular packets store information physically on themselves so that they cannot interfere with each other. Besides, the messenger molecules are assumed to be bioinactive, i.e., not easily corrupted or destroyed by natural processes. They are easily recognized by nanoreceptors such as molecular pumps or sorting rotors due to the special structure of these molecules containing a distinctive head [11].

The partially fluorinated polyethylene molecule [11] is a candidate for such messenger molecule since it has an information density of $d_i \sim 26$ bits/nm^3 which gives a distinguishably higher density when compared to DNA whose information density is $\sim$1 bit/nm^3 [11], which is widely suggested as an information storing molecule. Suggested in [12] for nanocomputer memory systems, a partially fluorinated polyethylene molecule is in the form, $\mathrm{CH_3(CHX)_nCH_2F}$, where X stands for H and F atoms representing 0 and 1 bits, respectively. These coded atoms are in one side of the chain while the other side of the chain is full of H atoms so that the receiver can recognize the coded side easily.

This molecule carries 50% H and 50% F atoms on the coded side of the molecule to equalize the molecular weight, hence the diffusion coefficient of all the intended symbols to reduce the analytical complexity. Still, for any source distribution, the ratio of the H and F atoms can be kept fixed doing an appropriate encoding at the nanotransmitter. However, any ratio of H and F atoms is feasible in the expense of unequal diffusion coefficients.

A partially fluorinated polyethylene molecule can carry l_m bits of information which is approximately given by $l_m \approx 4d_i/3\pi r^3$, where r is the spherical radius of the messenger molecule and d_i is the information density [11]. $n \neq l_m$ because of the allocation of some part of n bits for extra information about the message. In this study, to ease the decoding process at the receiver nanomachine, we allocate $n - l_m$ bits for message ID. Therefore, actual information density is slightly less than d_i. The head and tail structure of the molecule, $\mathrm{CH_3}$ and $\mathrm{CH_2F}$ forming the two ends of the molecule, provides a decoding order for the message.

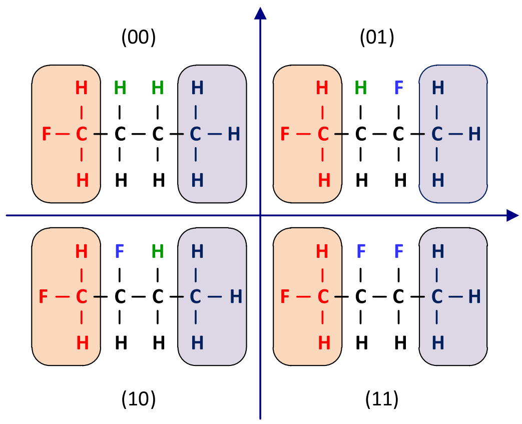

Fig. 1. Constellation diagram for QMoSK modulation, $n = 2$.

To increase the information carrying capacity of messengers, one needs larger molecules. However, larger molecules diffuse more slowly. According to the Einstein-Stokes relation [13], the diffusion coefficient D is inversely related with the size of the particles, i.e., $D = k_B T/6\pi\eta r$, where k_B is Boltzmann's constant, T is the absolute temperature, and η is the viscosity.

The information encoding process described here can exploit a molecular modulation technique such as molecule shift keying (MoSK) introduced in [14]. This modulation scheme requires 2^n different molecules to represent n bits of information. For the transmission of an intended symbol, one of these molecules are released by the transmitter and the receiver decodes the intended symbol according to the type of the received molecule. Inspired by [14], an $n = 2$ bit constellation diagram for Quadruple MoSK realized by fluorinated polyethylene is shown in Fig. 1.

B. Transmission Process

The transmitter nanomachine is assumed to have a spherical shape and the messenger molecules are released to the medium from the boundary of it. The emission process is uniformly distributed over this boundary called emission boundary.

The transmission strategy is chosen as *puffing of messengers*, i.e., instantaneous emission of puffs which are sets of released message molecules. Since the information is encoded in the type of molecule and not in its concentration, the transmitter does not need to continuously fill the medium with molecules which corresponds to continuous emission. In nature, puffing is usually used for modeling pheromone released in alarm situations such as presence of predators and enemies, injured conspecifics, exposure to toxic compounds, which require a sudden release of a limited amount of pheromones [22] as in the case of insect pheromone release [23], [24]. Thus, the transmitter does not prepare the molecules in advance, and does not store the molecules generated for future use.

When a nanomachine needs to transmit a single message, it generates puffs of N_M molecules. The probability of successful transmission of the message with just one puff is very low, therefore, for a single message N_P puffs of N_M molecules are sent. Accordingly, the transmission rate can be defined as

$$R^{(TX)} = \frac{l_m}{N_P T_M} \tag{1}$$

where T_M is the time required to prepare a puff and $N_P T_M$ to prepare a message.

C. Propagation Process

The position of a messenger molecule due to thermal noise as a function of time is modeled as a Brownian motion. The first hitting time of one molecule τ to a spherical surface at a distance d away from the emission boundary is distributed according to an inverse Gaussian probability density function [10], i.e.,

$$f_\tau(\tau) = \frac{d}{\sqrt{4\pi D\tau^3}} \exp\left(-\frac{(\nu\tau - d)^2}{4D\tau}\right), \quad \tau \geq 0 \tag{2}$$

where v is the mean drift velocity of the medium and D is the diffusion coefficient. The random variable τ can also be defined as the propagation delay of a single puff for a distance d.

D. Reception Process

A messenger molecule is assumed to be received at the time instant when it hits the boundary of the receiver. To calculate the reception rate, an interval of time beginning with the reception of the first message t_1 and ending with the reception of the $(k+1)$th message, t_{k+1}, is considered. The length of this time interval is $\Delta t = t_{k+1} - t_1$. Assume that $t_{k+1} - t_1 = \tau_{k+1} - \tau_1 + kN_P T_M$, where τ_{k+1} is the propagation delay for the $(k+1)$th message and τ_1 is the propagation delay for the first message. We assume that $E\{\tau_{k+1}\} = E\{\tau_1\}$ for all k regarding that the channel imposes the same expected delay to all messages. Hence, expected length of Δt can be calculated by $E\{\Delta t\} = kN_P T_M$.

During this time interval, kl_m information carrying bits are received. Thus, reception rate is expressed as

$$R^{(RX)} = \frac{l_m}{N_P T_M}. \tag{3}$$

Having a closed-form expression for rate, we try to obtain the *cumulative distribution function* (CDF) of delay. The probability of receiving the message is considered first.

If the reception boundary is the entire spherical surface that encapsulates the transmitter source, the probability of receiving the message before time t can be denoted by $P_M(t)$. It is the probability of the complementary event that none of $N_M N_P$ molecules released for one message is received before time t.

For each molecule of the ith puff, $F_\tau(t - iT_M)$ is the probability that it is received before time t, hence, $1 - F_\tau(t - iT_M)$ is the probability that it is not received. Thus, for that entire puff, $(1 - F_\tau(t - iT_M))^{N_M}$ is the probability that all N_M molecules of ith puff is not received before time t. Multiplying these probabilities for all puffs of a message, we obtain $\overline{P_M(t)} = \prod_{i=1}^{N_P} (1 - F_\tau(t - iT_M))^{N_M}$, representing the probability that none of $N_M N_P$ molecules is received before t. Finally, the probability that at least one molecule carrying the intended message is arrived, $P_M(t)$, is $1 - \overline{P_M(t)}$ and expressed

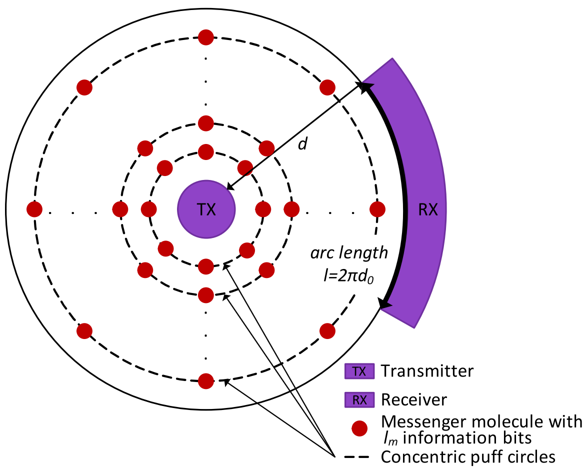

Fig. 2. Particle propagation and detection processes.

by

$$P_M(t) = 1 - \prod_{i=1}^{N_P} [1 - F_\tau(t - iT_M)]^{N_M} \tag{4}$$

where $F_\tau(\tau)$ is the CDF of τ. For simplicity, the initiation time of the message, i.e., release time of the first puff is taken as 0.

However, the reception boundary cannot encapsulate the transmitter source practically. Thus, there should be a probability P_d for detecting a messenger molecule when it is d away from the emission boundary. P_d can be expressed as the ratio of the length of receiving boundary, l $(=2\pi d_0$, for the shell shaped receiver), to the perimeter of the circle at distance d. P_d is expressed by

$$P_d = \begin{cases} 1, & \text{if } d \le d_0 \\ \dfrac{d_0}{d}, & \text{if } d > d_0 \end{cases}. \tag{5}$$

Up to a critical distance d_0, i.e., in the vicinity of the transmitter, the probability of reception is close to 1. However, when the receiver moves away beyond d_0, the probability of receiving falls below 1. As the receiver has a spherical shape, the receiving boundary cannot fit the arc with radius d completely as the shell shaped receiver shown in Fig. 2. Thus, d_0 is not directly equal to $l/2\pi$ but it is proportional with $l/2\pi$ in this case.

When N_P puffs are released, the probability of receiving the message as time goes to infinity becomes $P_r = 1-(1-P_d)^{N_P N_M}$. Then, to calculate the delay, we are conditioned that the message has to be received. Otherwise, we cannot define a finite delay for a nonreceived message. The probability $P_M(t)$ in (4) can be modified as a conditional probability, where M is the event that the message is received, i.e.,

$$P_M(t|\mathrm{M}) = \frac{1 - \prod_{i=1}^{N_P} [1 - P_d F_\tau(t - iT_M)]^{N_M}}{P_r}. \tag{6}$$

The probability that the message is received before t corresponds to the CDF of the message propagation delay, i.e., $F_{\tau_M}(\tau_M) = P_M(t|\mathrm{M})$. Since τ_M is a nonnegative random variable, the expected message propagation delay can be calculated by integrating the complementary CDF of τ_M,

$$E\{\tau_M|\mathrm{M}\} = \int_0^\infty (1 - F_{\tau_M}(t))\, dt. \tag{7}$$

For a single puff containing a single molecule, i.e., $N_M = 1$ and $N_P = 1$ in (6), the CDF of the delay, $F_{\tau_M}(t)$, becomes equal to $F_\tau(t)$ whose pdf is given in (2). Hence, the expected message propagation delay is equal to d/ν, the expected value of $F_\tau(t)$.

E. Information Decoding Process

Decoding of the messages is realized as the demodulation of the incoming molecule stream according to MoSK described in Section II-A. This demodulation is based on differentiating between different molecule types containing different numbers of H and F atoms. In nature, such a differentiating mechanism is found in pheromone receptors. For example, a very sensitive reception of pheromones exists in a male moth who can recognize potential mates, prey, and specific features of the environment such as food sources through the antennas placed on its olfactory system [25] which produces electrical signals in their neurons according to the type of the received pheromone. A similar system of antennas may be used by the receiver nanomachine which will process the information brought by the messenger molecule.

Another decoding mechanism, which is assumed to be used in this study, may be constructed to read the encoded information on the molecule, bit by bit using a convenient probe as suggested in [26]. The receiver nanomachine may be equipped with the specific C_5H_5B or $C_3H_3N_2B$ probe to identify the H or F atom using the difference in interaction energies between B atom of the probe and H/F atoms of the polyethylene. After decoding the message with this mechanism, the receiver identifies the message ID from the $n - l_m$ bits inserted in the message as suggested in Section II-A which will be the same for all N_M molecules of all N_P puffs carrying the same message.

A nanomachine may receive a message multiple times since there are redundant messenger molecules in the medium. Once a message is received and its ID is decoded, the subsequent molecules, which have the same ID, are not taken into consideration. The preparation time for one message is $N_P T_M$ as defined in Section II-B. To reduce the energy for decoding the redundant molecules, the receiver waits during $T_{\text{wait}} = \alpha N_P T_M$ $(\alpha > 1)$, after the reception of the first message since a second one cannot be generated by the transmitter in a time duration of $N_P T_M$.

III. Rate-Delay Tradeoff With Network Coding

In this section, a mathematical model is derived to characterize the rate-delay tradeoff of a molecular nanonetwork which also describes a simple network coding mechanism that improves the rate-delay performance of this nanonetwork. Consider a relay network containing a Nano-Relay as shown in Fig. 3, where Nano-Alice and Nano-Bob need to send each other a message.

Nano-Alice and Nano-Bob function as both nanotransmitter and nanoreceiver realizing all the five main processes mentioned in Section II. Assume that Nano-Alice and Nano-Bob are not

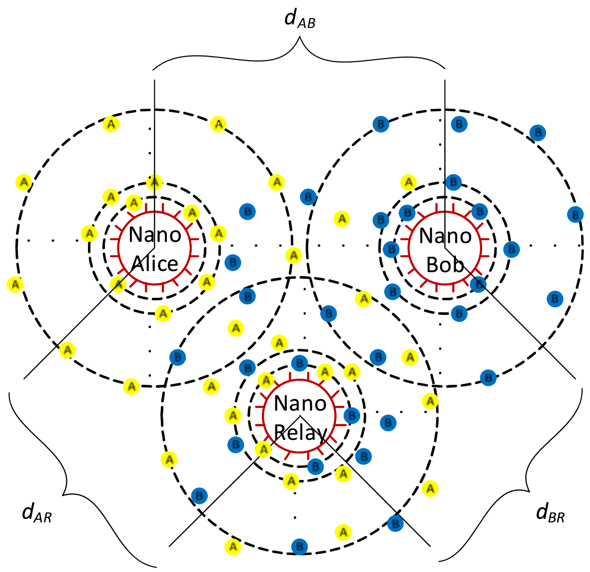

Fig. 3. Simple uncoded network mechanism.

in the communication range of each other but in the communication range of Nano-Relay, i.e., $d_{AR} < d_0, d_{RB} < d_0, 2d_0 > d_{AB} > d_0$. Nano-Relay can operate both as a nanotransmitter and a nanoreceiver. Additionally, Nano-Relay combines the incoming messages from Nano-Alice and Nano-Bob and determines whether to generate new molecules or relay the incoming molecules.

In order to improve the rate-delay characteristics of this system, in the second part of this section, we introduce a basic network coding mechanism where Nano-Relay XORs the messages coming from Nano-Alice and Nano-Bob. Although there is no study on XOR operation for fluorinated polyethylene, an XOR gate can be implemented at the molecular level by pseudorotaxane [34]. A molecular XOR scheme can be generated such that Nano-Relay combines the information coming from Nano-Alice and Nano-Bob by XORing H and F atoms sequentially, i.e., starting from head of the molecule until its tail, which is in fact similar to binary XOR operation on a string of zeros and ones. More specifically, if the message strings coming from both Nano-Alice and Nano-Bob contain the same atom to be XORed, Nano-Relay outputs H. Otherwise, it transmits F. Hence, knowing the bit they sent, Nano-Alice and Nano-Bob decide what was sent by the other.

In this scheme, the ultimate goal is that Nano-Alice and Nano-Bob exchange a pair of messages. Without network coding, Nano-Alice sends its message to Nano-Relay which forwards it to Nano-Bob and Nano-Bob sends its message to Nano-Relay which forwards it to Nano-Alice. Thus, we have four transmissions in total. When the network coding mechanism is considered, Nano-Alice and Nano-Bob send their messages to Nano-Relay which XORs and sends the combined message back to them which requires a total of three transmissions instead of four. As Nano-Alice and Nano-Bob know their sent message, they can decode Nano-Relay's message and extract the messages of their respective partners. Hence, the molecular network coding can be used for increasing the rate since the same information is sent now with less number of transmission, i.e., in a shorter time interval.

A. Rate-Delay Tradeoff for an Uncoded Case

Assume that Nano-Alice and Nano-Bob start transmitting their messages at the same time instant. Both of them do not know about the position of the other and release N_P puffs of messenger molecules into the communication medium. Since the propagation delay for a Brownian message is a random variable, Nano-Relay receives messages from Nano-Alice and Nano-Bob at random time instants. The forwarding procedure for a message starts when it is received by Nano-Relay. However if a second message arrives during the transmission of the first, Nano-Relay puts it in the queue and this second message waits until the transmission of the first is finished. The waiting time of a message in the queue is denoted as T_q.

Let A and B be the messages of Nano-Alice and Nano-Bob, respectively. Both A and B can reach their destinations directly or from the path over Nano-Relay. Then, the expected delay $E\{T_D\}$ for a message to reach its destination can be calculated as

$$E\{T_D\} = E\{T_D|AB\}\, P(AB) + E\{T_D|\overline{AB}\}\, P(\overline{AB}) \quad (8)$$

where AB is the event when the same message is transferred on both Nano-Relay and the direct path between Nano-Alice and Nano-Bob, simultaneously. $\overline{AB}$ represents the complement event when the message is transferred on only Nano-Relay.

The probability AB event is $P(AB) = 1-(1-d_0/d_{AB})^{N_P}$. If the message fails to reach its destination on the direct path ($\overline{AB}$ case), the delay is completely determined by the transmission path over Nano-Relay, which is given by $E\{T_D|\overline{AB}\} = E\{T_{ARB}\}$, where T_{ARB} is the delay for the path ARB. Otherwise, when AB event occurs, the delay is the minimum of time delays to which the message molecules are exposed for paths ARB and AB, $E\{T_D|AB\} = E\{\min(T_{AB}, T_{ARB})\}$, where T_{AB} is the delay for the path AB.

$E\{T_D|AB\}$ is upper bounded by $E\{T_{AB}\}$ since $E\{T_{AB}\} < E\{T_{ARB}\}$ due to the triangle inequality

$$E\{T_D|AB\} < E\{T_{AB}\} = E\{\tau_M\}. \quad (9)$$

Then, the expected message delay between A and B using (7) is

$$E\{\tau_M\} = \int_0^\infty \left[\frac{\prod_{i=1}^{N_P}(1-P_d F_\tau(t-iT_M))^{N_M} - (1-P_d)^{N_P N_M}}{1-(1-P_d)^{N_P N_M}}\right] dt. \quad (10)$$

Nevertheless, it is troublesome to find a closed-form expression using (10). Thus, we provide the upper and lower bounds for this integral to show the behavior of delay. A lower bound for the expected message delay between A and B is obtained as

$$E\{\tau_M\} > \frac{1-(1-P_d)^{N_P N_M+1} - P_d(N_P N_M+1)(1-P_d)^{N_P N_M}}{\xi P_d (N_P N_M+1) P_r}. \quad (11)$$

To arrive to this bound let us define a new CDF, $F_{\tau^{(u)}}(t)$, which is the CDF of a uniform random variable $\tau^{(u)}$,

$$F_{\tau^{(u)}}(t) = \begin{cases} t/\xi, & \text{if } t \in (0,\xi) \\ 1, & \text{if } t \geq \xi \\ 0, & \text{else} \end{cases} \tag{12}$$

where ξ is mode of the pdf of τ, i.e., the point where the peak of the pdf occurs, which can be calculated by differentiating $f_\tau(t)$ and equating to zero, i.e., $\xi = (-3D + \sqrt{9D^2 + d^2 v^2})/v^2 > 0$. Note that compared to the infinite duration pdf of τ, which is inverse Gaussian distribution, we observe that the uniformly distributed $\tau^{(u)}$ has a much narrower pdf. However, its density is greater than $f_\tau(t)$ for $t \in (0, \xi)$. Hence, the CDF $F_{\tau^{(u)}}(t)$ is larger than $F_\tau(t)$ for every t in $(0, \infty)$. Thus, uniform distribution approximation of $f_\tau(t)$ yields an upper bound on the propagation delay pdf, which, in turn, yields the lower bound for $E\{\tau_M\}$ in (11) calculated by substituting (12) into $F_\tau(t - iT_M)$ for each i in (10).

Similar to lower bound in (11), an upper bound is obtained as

$$E\{\tau_M\} < -\frac{(1-P_d)^{N_P N_M}}{P_r} + \frac{(1-P_d N_P N_M/\mu)^{N_P N_M+1} - (1-P_d(N_P N_M+\mu)/\mu)^{N_P N_M+1}}{\mu P_d (N_P N_M + 1) P_r}. \tag{13}$$

To get this bound, we define a new CDF, $F_{\tau^{(v)}}(t)$, which is the CDF of a uniform random variable $\tau^{(v)}$,

$$F_{\tau^{(v)}}(t) = \begin{cases} t/\mu, & \text{if } t \in (0,\mu) \\ 1, & \text{if } t \geq \mu \\ 0, & \text{else} \end{cases} \tag{14}$$

where μ is the expected value of the pdf of τ. Note that for the expected value, μ, $F_\tau(t)$ reaches 0.99 which is sufficiently close to 1 so that we can assume $F_\tau(t)$ is 1 for $t > \mu$. Besides, $F_{\tau^{(v)}}(t)$ increases very slowly compared to $F_\tau(t)$ for $t \in (0, \mu)$. Hence, the CDF $F_{\tau^{(v)}}(t)$ is smaller than $F_\tau(t)$ for every t value in $\in(0, \infty)$. To simplify (10), we replace $F_\tau(t - iT_M)$ by $F_{\tau^{(v)}}(t - N_P T_M)$ for all i, since $F_{\tau^{(v)}}(t - N_P T_M) \leq F_\tau(t - N_P T_M) \leq F_\tau(t - iT_M)$ for all i. Thus, this approximation yields a lower bound on the propagation delay CDF, which, in turn, yields the upper bound for $E\{\tau_M\}$ in (13). Using (9), we obtain

$$E\{T_D\} < E\{T_{AB}\} P(AB) + (E\{T_{ARB}\} + E\{T_q\}) P(\overline{AB}). \tag{15}$$

$E\{T_q\}$ is included in (15) to represent the expected queuing delay for message A in the Nano-Relay defined in Section III-A.

First, assume that only messages A and B of Alice and Bob, respectively, need to be forwarded by Nano-Relay without coding. In that case, if A is received during the transmission of the message B, the message A waits a period of time, $E\{T_q{}^{(\overline{C})}\}$, which is expressed by $E\{T_q{}^{(\overline{C})}\} = P\{Q^{(\overline{C})}\} E\{T_q{}^{(\overline{C})} | Q^{(\overline{C})}\}$, where $Q^{(\overline{C})}$ is the event that A is received in the transmission period of B. The probability of queueing in an uncoded case is

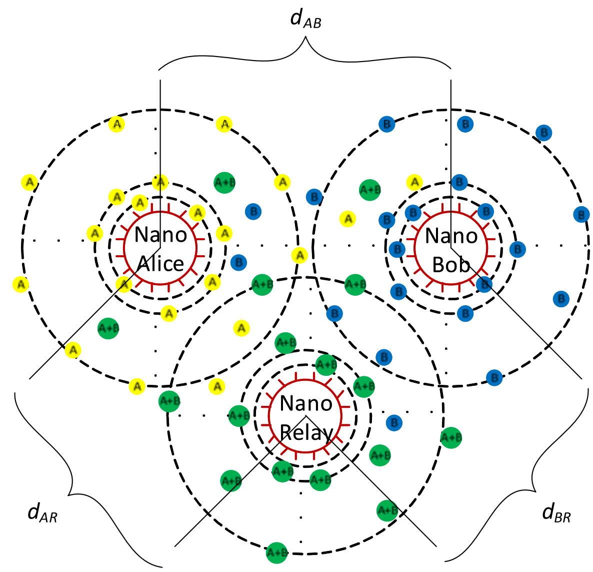

Fig. 4. Simple network coding mechanism.

$$P\left\{Q^{(\overline{C})}\right\} = Pr\{N_P T_M > \tau_A - \tau_B > 0\} \tag{16}$$

where τ_A and τ_B are the respective propagation delays of messages A and B. We assume that puff propagation delays are exponentially distributed with mean d/ν.

For exponentially distributed propagation delays, the probability $P\{Q^{(\overline{C})}\}$ is given by

$$P\left\{Q^{(\overline{C})}\right\} = \frac{d_{AR}}{d_{AR} + d_{BR}} \left(1 - \exp\left(-\frac{\nu N_P^2 T_M}{d_{AR}}\right)\right). \tag{17}$$

Suppose that message streams from Nano-Alice and Nano-Bob have Poisson arrivals with rates α and β, respectively. Then, Nano-Relay can be modeled as an M/G/1 server having a service time distribution with mean μ and variance σ^2. Thus, the expected queueing delay can be derived using the *Pollaczek-Khintchine formula* [29]. Specifically, Nano-Relay becomes an M/D/1 server when network coding is not allowed, i.e., direct forwarding.

For M/D/1 case, the relay throughput is constant with rate $1/N_P T_M$ messages per unit time and the expected queueing for an arbitrary message can be calculated by [29] as

$$E\left\{T_q | Q^{(\overline{C})}\right\} = \frac{1}{2} \frac{(\alpha+\beta) N_P^2 T_M^2}{1 - (\alpha+\beta) N_P T_M}. \tag{18}$$

Similar to the reception rate calculation in Section II-D, reception rate of Nano-Alice's messages at Nano-Bob can be calculated as

$$R_{\overline{C}}^{(RX)} = \frac{l_m}{N_P T_M}. \tag{19}$$

B. Rate-Delay Tradeoff for a Network Coded Case

Now, consider the case when Nano-Relay uses a network coding mechanism, which is shown in Fig. 4. When Nano-Relay receives a message, it starts waiting T_W s for the other message to arrive before transmitting the received message. If the other message arrives within T_W s, Nano-Relay starts transmitting the XORed version of two messages. Otherwise, Nano-Relay transmits messages separately.

If Nano-Relay forwards messages with the network coding mechanism, the expected queuing delay for message A becomes

$$E\left\{T_q^{(C)}\right\} = P\left\{W^{(C)}\right\} E\left\{T_q^{(C)}|W\right\} + P\left\{\overline{W}^{(C)}\right\} T_W \quad (20)$$

where W is the event when the message B arrives within the waiting time T_W in a coded case with probability $P\left\{W^{(C)}\right\}$, calculated assuming exponential propagation delays as

$$P\left\{W^{(C)}\right\} = \frac{d_{BR}}{d_{BR}+d_{BR}}\left(1-\exp\left(-\frac{\nu N_P T_W}{d_{BR}}\right)\right). \quad (21)$$

Even when each of Nano-Alice and Nano-Bob generates one single message, the advantage of network coding is reflected as reduced resource consumption in Nano-Relay. However, if both sources generate message streams, then the forwarding efficiency of Nano-Relay can significantly affect the delay. When both sources continously emit puffs of molecules, Nano-Relay continously combines the molecules. Since there are always molecules ready to combine arriving from the other source, no molecule waits up to T_W for its conjugate to arrive. Hence, the total waiting time which adversely affects the delay, decreases.

In the network coding case, the relay throughput can be assumed to have a bimodal distribution. Assume that only messages transmitted at the same time can be coded with each other. When a message is going to be transmitted and its conjugate message is in the queuing buffer, then these messages can be forwarded together meaning that the relay throughput is $2/N_P T_M$ messages per unit time. Otherwise, they are transmitted with rate $1/N_P T_M$ messages per unit time.

Similar to the uncoded case, the expected queueing delay for an arbitrary message in the network-coded case can be calculated by

$$E\left\{T_q^{(C)}|W\right\} = \frac{(1-0.75P_{AXB})(\alpha+\beta)N_P^2 T_M^2}{2\left(1-(\alpha+\beta)(1-0.5P_{AXB})N_P T_M\right)} \quad (22)$$

where P_{AXB} is the probability of coding the messages A and B.

Note that as the probability P_{AXB} increases, $E\{T_q\}$, i.e., the expected queueing delay, decreases. However, the probability P_{AXB} is also a function of the queueing delay T_q since longer queueing delays increase the chance for coding of conjugate messages. Therefore, the probability P_{AXB} is defined as $P_{AXB} = Pr\{|\tau_A - \tau_B| < T_q\}$, where τ_A and τ_B are the reception times of conjugate messages from Nano-Alice and Nano-Bob.

Similar to the reception rate calculation in Section II-D, reception rate of Nano-Alice's messages at Nano-Bob can be calculated as

$$R_C^{(RX)} = \frac{l_m}{N_P T_M}\left(2P\left\{W^C\right\} + (1-P\{W^C\})\right). \quad (23)$$

TABLE I
SIMULATION PARAMETERS

Parameter	**Symbol**	**Value**
Diffusion coefficient	D	$2.2 \times 10^{-11}\ m^2/s$
Drift velocity	v	$0.2 \times 10^{-9}\ m/s$
Distance b/w two transceivers	d	$10^{-5}\ m$
Puff preparation time	T_M	$10^{-3}\ s$
Probability of coding messages	P_{AXB}	1
Poisson arrival rate of Alice	α	$0.1\ s^{-1}$
Poisson arrival rate of Bob	β	$0.1\ s^{-1}$
Distance b/w Alice and Relay	d_{AR}	$10^{-6}\ m$
Distance b/w Bob and Relay	d_{BR}	$10^{-6}\ m$
Distance b/w Alice and Bob	d_{AB}	$2 \times 10^{-6}\ m$
Area of perfect reception	A	$10^{-10}\ m^2$
Number of molecules in a puff	N_M	10

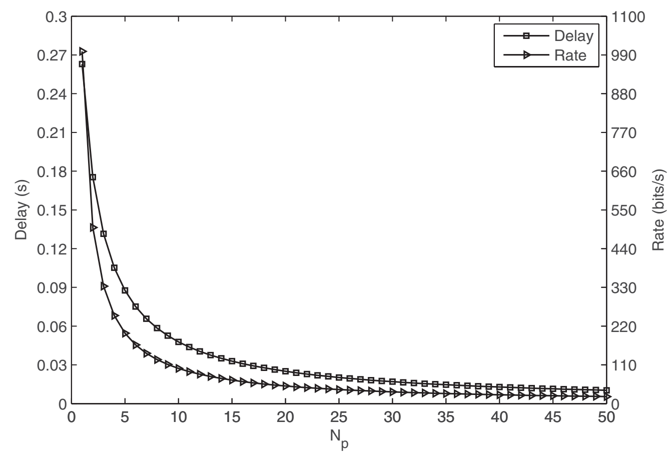

Fig. 5. Delay and rate characteristics with N_P.

IV. SIMULATIONS

In this section, we evaluate rate and delay expressions found in Section II and III with the simulation parameters given in Table I, chosen in agreement with [11]. Then, the uncoded and the network coded cases are compared to reveal the rate-delay tradeoff.

A. Simulation for an Uncoded Case

We investigate the rate-delay tradeoff of the uncoded case without a relay in Fig. 5 to illustrate the decaying trend of rate and delay with increasing N_P. The rate expression in (3) is utilized to evaluate the rate variation. Our analysis is not based on the exact expressions of the delay but on the lower and upper bounds, given in (11) and (13). Although the two bounds follow the same trend, the lower bound is far beyond the realistic propagation delays in molecular domain, hence, upper bound (13) is preferred.

On the one hand, for a single message, as the number of puffs N_P increases, the preparation time for the message increases proportionally. Therefore, the transmission rate $R^{(TX)}$ and the reception rate $R^{(RX)}$ increase. On the other hand, increasing N_P augments the message reception probability, causing a descent in expected message propagation delay $E\{\tau_M\}$. Thus, there is a tradeoff between the expected message propagation delay $E\{\tau_M\}$ and the expected reception rate $R^{(RX)}$. These results

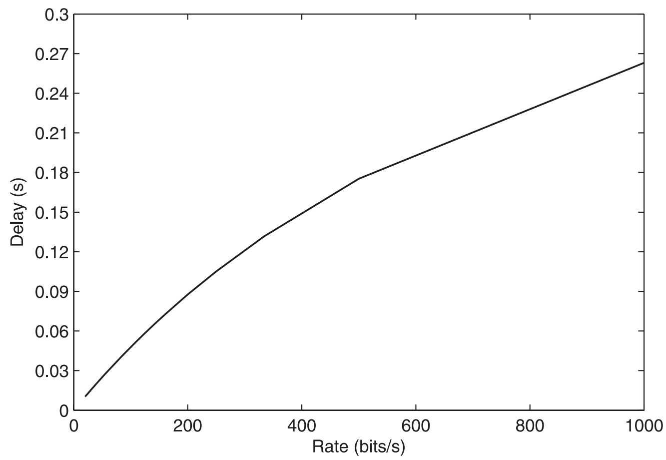

Fig. 6. Rate versus delay analysis.

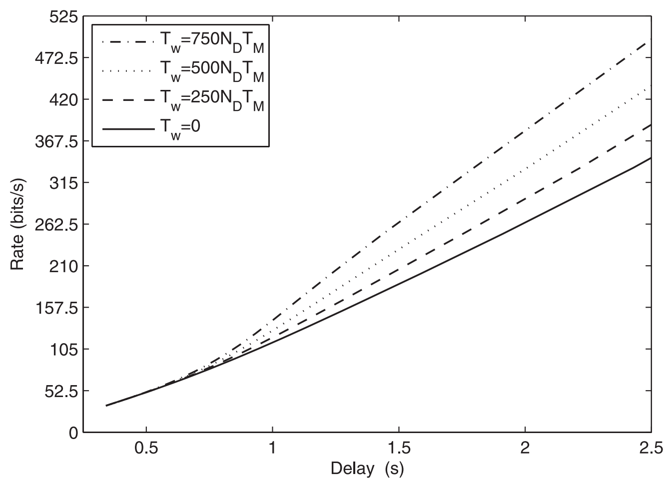

Fig. 7. Rate versus delay analysis in uncoded and coded network cases.

are also intuitively expected from (3), (11), and (13). The tradeoff between rate and delay is illustrated in Fig. 6. This rate-delay tradeoff analysis is crucial for designing an efficient molecular communication network. An important application of molecular networks is molecular computers which will be an alternative for electronic computers in the future [27] due to the hundred times smaller size of molecules with respect to silicon chips of electronic computers and the high parallel computing capacity of molecular computers [28]. The rate and delay characteristics of different molecular communication techniques will be essential criteria for the design of these molecular computers which will boost the computing power to ten-thousandfold of electronic computers. Especially, in gene regulatory applications, molecular computers doing DNA computations are highly investigated in various studies such as [30] and [31].

B. Simulation for a Network Coded Case

In Fig. 7, reception rates with respect to delay of both uncoded and network coded cases with different waiting times in Nano-Relay, denoted by T_W, are illustrated. $T_W = 0$ represents the uncoded case. On the one hand, as T_W increases, the waiting interval for conjugate messages increases, which, in turn, increases the probability of coding. Therefore, total delay increases due to the extra delay introduced by Nano-Relay before coding takes place. On the other hand, as the probability of coding increases, the reception rate increases since Nano-Relay combines the incoming messages to decrease the number of transmitted messages. As illustrated in Fig. 7, by increasing the waiting time T_W, 40% higher reception rate compared to the uncoded case, i.e, $T_W = 0$, is achievable for a given delay yielding the advantage of using network coding in molecular nanonetworks.

The network coding technique is a beneficial tool to overcome long propagation delay problem for molecular communication in vast different applications. For medical applications, to improve the intervention time of nanorobots placed in the human body described in [32], the molecular communication between them may be accelerated by network coding in order to identify the tumor cells effectively. Another medical application can be stated as the regulation of the behaviors of engineered bacteria used in cancer therapy [33]. These bacteria form quorum sensing networks by communicating via signaling molecules to sense the environment of a tumourous cell, invade that cell and release cytotoxic agents. The efficient operation of these bacteria arises from their proper synchronization which may be established by a low delay molecular network.

V. Conclusion

Molecular communication is a promising field open to evolution because of its feasibility in a vast variety of fields, such as environment, industry, military, and especially biomedicine. Biomedical applications utilize messenger-based approaches that have crucial roles in intervening in biological processes to artificially control biosystems. For this reason, we build our analysis on a specific case of messenger-based molecular communication model. First, we model the puff propagation using a Brownian motion model. Next, using this model, the mathematical relation between reception rate and message delay is extracted to justify the tradeoff between them. Then, this model is applied to a simple nanonetwork in two different cases, namely, uncoded and network coded cases. Finally, the expressions of rate and delay are evaluated for both cases.

In brief, our analysis shows that high data rate and negligible propagation delay cannot be achieved simultaneously as opposed to an ideal communication system. The tradeoff should be exploited in delay or rate sensitive molecular nanoscale applications. This pioneering study constitutes a basis for rate and delay optimization of future nanomolecular frameworks.

References

[1] I. F. Akyildiz, F. Brunetti, and C. Blázquez, "Nanonetworks: A new communication paradigm," *Comput. Netw.*, vol. 52, no. 12, pp. 2260–2279, 2008

[2] T. Nakano and J.-Q. Liu, "Design and analysis of molecular relay channels: An information theoretic approach," *IEEE Trans. Nanobiosci.*, vol. 9, no. 3, pp. 213–221, Sep. 2010.

[3] M. Mukai, K. Maruo, J. Kikuchi, Y. Sasaki, S. Hiyama, Y. Moritani, and T. Suda, "Propagation and amplification of molecular information using a photo-responsive molecular switch," *Supramol. Chem.*, vol. 21, no. 3–4, pp. 284–291, 2009.

[4] K. Yasuhara, Z. Wang, T. Ishikawa, J. Kikuchi, Y. Sasaki, S. Hiyama, Y. Moritani, and T. Suda, "Specific delivery of transport vesicles mediated by complementary recognition of DNA signals with membrane-bound oligonucleotide lipids," *Supramol. Chem.*, vol. 23, no. 3–4, pp. 218–225, 2011.
[5] Y. Sasaki, Y. Shioyama, W. Tian, J. Kikuchi, S. Hiyama, Y. Moritani, and T. Suda, "A nano sensory device fabricated on a liposome for detection of chemical signals," *Biotechnol. Bioeng.*, vol. 105, no. 1, pp. 37–43, 2010.
[6] M. Pierobon and I. F. Akyildiz, "A physical end-to-end model for molecular communication in nanonetworks," *IEEE J. Sel. Areas Commun.*, vol. 28, no. 4, pp. 602–611, May 2010.
[7] B. Atakan and O. B. Akan, "An information theoretical approach for molecular communication," in *Proc. ICST/ACM Bionetics*, Dec. 2007, pp. 33–40.
[8] D. Arifler, "Capacity analysis of a diffusion-based short-range molecular nano-communication channel," *Comput. Netw.*, vol. 55, no. 6, pp. 1426–1434, 2011.
[9] M. Pierobon and I. F. Akyildiz, "Diffusion-based noise analysis for molecular communication in nanonetworks," *IEEE Trans. Signal Process.*, vol. 59, no. 6, pp. 2532–2547, Jun. 2011.
[10] R. S. Adve and A.W. Eckford, "Molecular communication using brownian motion with drift," *IEEE Trans. Nanobiosci.*, vol. 11, no. 2, pp. 89–99, Jun. 2012.
[11] R. A. Freitas, *Nanomedicine, Volume I: Basic Capabilities*. Georgetown, TX, USA: Landes Bioscience, 1999, pp. 178–180.
[12] K. Eric Drexler, *Nanosystems: Molecular Machinery, Manufacturing, and Computation*. New York, USA: Wiley, 1992.
[13] S. Lindsay, *Introduction to Nanoscience*. Oxford, U.K.: Oxford Univ. Press, 2009.
[14] M. S. Kuran, H. B. Yilmaz, T. Tugcu, and I. F. Akyildiz, "Modulation techniques for communication via diffusion in nanonetworks," in *Proc. IEEE Int. Conf. Commun.*, Jun. 2011, pp. 1–5.
[15] T. D. Schneider, "Sequence logos, machine/channel capacity, Maxwell's demon, and molecular computers: A review of the theory of molecular machine," *Nanotechnology*, vol. 5, no. 1, pp. 1–18, 1994.
[16] Y. Li, M. Chiang, R. Calderbank, and S. N. Diggavi, "Optimal rate-reliability-delay tradeoff in networks with composite links," *IEEE Trans. Commun.*, vol. 57, no. 5, pp. 1390–1401, May 2009.
[17] M. Vehkaperä and M. Médard, "A throughput-delay trade-Off in packetized systems with erasures," in *Proc. Int. Symp. Inf. Theory*, Sep. 2005, pp. 1858–1862.
[18] J. M. Walsh, S. Weber, and C. W. Maina, "Optimal rate delay tradeoffs for multipath routed and network coded networks," in *Proc. Int. Symp. Inf. Theory*, Jul. 2008, pp. 682–686.
[19] T. F. Zuck and J. G. Riess, "Current status of injectable oxygen carriers," *Crit. Rev. Clin. Lab. Sci.*, vol. 31, no. 4, pp. 295–324, 1994.
[20] B. Atakan, S. Balasubramaniam, and O. B. Akan, "Body area nanonetworks with molecular communications in nanomedicine," *IEEE Commun. Mag.*, vol. 50, no. 1, pp. 28–34, Jan. 2012.
[21] L. Parcerisa and I. F. Akyildiz, "Molecular communication options for long range nanonetworks," *Comput. Netw.*, vol. 53, no. 16, pp. 2753–2766, 2009.
[22] T. D. Wyatt, *Pheromones and Animal Behaviour: Communication By Smell and Taste*. Cambridge, U.K.: Cambridge Univ. Press, 2003, pp. 9–10.
[23] T. Strand, B. Lamb, H. Thistle, E. Allwine, and H. Peterson, "A simple model for simulation of insect pheromone dispersion within forest canopies," *Ecol. Model.*, vol. 220, no. 5, pp. 640–656, 2009.
[24] J. Law and F. Regnier, "Pheromones," *Annu. Rev. Biochem.*, vol. 40, pp. 533–548, 1971.
[25] W. Leal, *Pheromone Reception, Topics in Current Chemistry*. Heidelberg/Berlin, Germany: Springer-Verlag, 2005.
[26] C. W. Bauschlicher, Jr., A. Ricca, and R. Merkle, "Chemical storage of data," *Nanotechnology*, vol. 8, no. 1, pp. 1–5, 1997.
[27] M. S. Livstone, D. Noort, and L. F. Landweber, "Molecular computing revisited: A moore's law?" *Trends Biotechnol.*, vol. 21, no. 3, pp. 98–101, 2003.
[28] T. Munakata, "Beyond silicon: New computing paradigms," *Commun. ACM*, vol. 50, no. 9, pp. 30–34, 2007.
[29] A. Y. Khintchine, "Mathematical theory of a stationary queue," *Mathematicheskii Sbornik*, vol. 39, pp. 64–100, 1930.
[30] Y. Benenson, B. Gil, U. Ben-Dor, R. Adar, and E. Shapiro, "An autonomous molecular computer for logical control of gene expression," *Nature*, no. 429, pp. 423–429, 2004.
[31] J. L. Richard and E. B. Baum, "DNA based computers," in *Proc. DIMACS Workshop*, 1995, vol. 27.
[32] A. Cavalcanti, T. Hogg, B. Shirinzadeh, and H. C. Liaw, "Nanorobot communication techniques: A comprehensive tutorial," in *Proc. IEEE ICARCV 2006*, Singapore, Dec., pp. 1–6.
[33] J. C. Anderson, E. J. Clarke, A. P. Arkin, and C. A. Voigt, "Environmentally controlled invasion of cancer cells by engineered bacteria," *J. Mol. Biol.*, vol. 355, no. 4, pp. 619–627, 2005.
[34] A. Credi, V. Balzani, S. J. Langford, and J. F. Stoddart, "Logic operations at the molecular level. An XOR gate based on a molecular machine," *J. Amer. Chem. Soc.*, vol. 119, no. 11, pp. 2679–2681, 1997.

Bige D. Unluturk (S'12) completed her high school education in Galatasaray High School, Istanbul, Turkey, in 2007. She received the B.Sc. degree in electrical and electronics engineering from Middle East Technical University,Ankara, Turkey, and is currently working toward the M.Sc degree at the Department of Electrical and Computer Engineering, Koc University, Istanbul, Turkey.

She is currently a Research Assistant at Next-Generation Wireless Communication Laboratory.

Derya Malak (S'11) received the B.Sc. degree in electrical and electronics engineering from Middle East Technical University, Ankara, Turkey, in 2010, and working toward the M.Sc. degree at the Department of Electrical and Electronics Engineering, Koc University, Istanbul, Turkey.

She is currently a Research Assistant in the Next-generation and Wireless Communication Laboratory. Her current research interests include nanoscale communication, intrabody molecular communication networks, and network information theory.

Ozgur B. Akan (M'00–SM'07) received the Ph.D. degree in electrical and computer engineering from Georgia Institute of Technology, Atlanta, USA, in 2004.

He is a Full Professor with the Department of Electrical and Electronics Engineering and the Director of the Next-Generation and Wireless Communications Laboratory, Koc University, Istanbul, Turkey. His current research interests include wireless communications, nanoscale and molecular communications, and information theory.

Dr. Akan is currently the General Cochair of ACM MOBICOM 2012 and IEEE MoNaCom 2012. He is also the Technical Program Committee Cochair of IEEE ISCC 2012. He is an Associate Editor of the IEEE TRANSACTIONS ON VEHICULAR TECHNOLOGY, the *International Journal of Communication Systems* (Wiley), and the *Nano Communication Networks Journal* (Elsevier).