An Information Theoretical Study on Nanoscale Communication Channels with Molecule Diversity

by

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ABSTRACT

Molecular communication is a promising technique to establish communication at nanoscale in which molecules are used to carry messages between nanomachines. It has many applications areas such as environmental applications, which include water and air pollution control, industrial applications, which include development of intelligent materials, nano-processors and nano-memory, and biomedical applications, which are drug delivery, disease diagnosis&treatment and health monitoring. In this thesis, we introduce a new model for molecular communication which exploits molecule diversity. An information theoretical analysis of this channel is conducted to investigate the rate-delay trade-off, the capacity and the bit error rate. Our aim in this thesis is to find the feasible conditions and techniques to realize a molecular communication system. Furthermore, we derived analogies between the conventional electromagnetic communications and the emerging molecular communication fields to exploit the techniques used in conventional networks such as network coding and forward error correction for optimizing the performance of molecular networks.

ÖZET

Moleküler haberleşme, nanomakinalar arasındaki mesajların moleküller aracılığıyla taşındığı gelecek vaat eden nano-ölçekli bir haberleşme tekniğidir. Çok sayıda olası kullanım alanından bazılarışunlardır: su ve hava kirliliği kontrol gibi çevresel uygulamalar; akıllı malzemeler, nano-işlemci ve nano-belleklerin üretimi gibi endüstriyel uygulamalar; ilaç dağıtımı, çeşitli hastalıkların tanı ve tedavisi, sağlık izleme gibi biomedikal uygulamalar. Bu tezde, molekül çeşitliliğini kullanan yeni bir moleküler haberleşme modeli tanıtılmaktadır. Bu kanalın bilgi aktarım hızıve gecikme ödünleşmesi, kanal kapasitesi ve bit hata oranını incelemek için kanalın bilgi kuramsal analizi yapılmıştır. Bu tezdeki amacımız, moleküler haberleşme sistemlerini gerçekleyebilmek için gerekli elverişli durumlarıve teknikleri ortaya çıkarmaktır. Ayrıca, geleneksel elektromanyetik haberleşme ile hızla gelişen moleküler haberleşme arasında analojiler kurarak geleneksel ağlarda kullanılan ağ kodlaması, gönderme yönünde hata düzeltimi gibi tekniklerin moleküler ağlara uygulanması amaçlanmaktadır.

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ABBREVIATIONS

ARQ	Automatic Repeat Request
BER	Bit Error Rate
CDF	Cumulative Distribution Function
FDA	US Food and Drug Administration
FEC	Forward Error Correction
FRET	Frequency Resonant Energy Transfer
ICT	Information and Communication Technologies
ID	Identifier
ISI	Inter-symbol Interference
MEMS	Micro Electro-Mechanical Systems
RX	Receiver
TX	Transmitter

Chapter 1

INTRODUCTION

Molecular communication constitutes a novel communication paradigm in which the information is encoded on and decoded from the molecules [1]. Considering the growth in the fabrication of nanomachines for diverse applications spanning biomedical, industrial, environmental and military applications [2], it is vital to establish a communication architecture to allow nanomachines to collaborate with each other. To respond to this need, we proposed a communication model where the information is encoded on fluorinated polyethylene molecule and tried to transfer the knowledge from classical ICT based on electromagnetic communications to molecular communication domain by adapting some techniques to nanonetwork environment such as network coding and error compensation. Firstly, we investigated the rate-delay tradeoff of molecular nanonetworks using this model. A basic network coding mechanism is also proposed to improve the rate-delay tradeoff. Furthermore, slightly modifying this communication model for an application in human body, we derived the capacity of a molecular communication channel using this model. By varying the parameters, we optimized the number of bits that can be encoded on a polyethylene molecule. Besides, we investigated the bit error rate-power tradeoff for this channel and proposed using Forward Error Correction to improve.

1.1 Molecular Communication

The recent advances in nanotechnology promise new solutions for a wide area of applications such as biomedical, industrial and military fields. Nanomachines are considered as the most basic functional units which are able of performing very simple tasks in a range of few hundred nanometers. These nanomachines form nanonetworks by collaborating ans sharing information in order to accomplish macroscale tasks [1]. Using traditional electromagnetic wave communication is limited for nanonetworks because of power constraints and physical limitations in the size and nature of nanomachines [3]. Thus, a novel communication paradigm appropriate for nanoscale, molecular communication, has emerged which demands novel solutions such as molecular transceiver design, channel models and communication architectures and protocols.

The idea of using molecules for communication purposes is first proposed in [5] and the first framework for molecular communication is established in [4] in 2005. Molecular communication is based on encoding the information on concentration/type/arrival time of molecules released by the transmitter nanomachines. Receiver nanomachines decode the information encoded on the molecules by biochemical reactions.

Some of the molecular communication techniques are diffusion based molecular communication [6, 7, 8, 60], calcium signalling [10, 11], bacteria nanonetworks [12], and Förster resonance energy transfer [13].

Diffusion based molecular communication is the most general architecture. Molecules are released from the transmitter nanomachine and they are assumed to propagate from the transmitter to the receiver by Fick's Law of diffusion. Generally, their random motion is modelled as a Brownian motion.

For calcium signalling, the information is encoded in the concentration of the

calcium ions. When the concentration of calcium ions are varied in the vicinity of sensitive cells such as a neuron or a cardiomyocyte this variation cause a change in the electrical charge of the membrane and the received signal is tranduced into an electric signal.

In bacteria communication, a bacterium transmits a message by releasing information molecules in the medium where the bacteria population lies. Another bacteria in the medium captures the propagating molecule released by the first bacteria and receives the message.

Förster Resonant Energy Transfer (FRET) is a nonradiative energy transfer process between uorescent molecules based on the dipole-dipole interactions of molecules. Low dependence on the environmental factors, controllability of its basic parameters, and relatively wide transfer range make FRET a promising candidate to be used for high-rate nanoscale wireless communications technique.

1.2 Research Objectives and Solutions

Our research objectives and suggested solutions are explained in this section.

1.2.1 Rate-Delay Tradeoff with Network Coding in Molecular Nanonetworks

Molecular communication differentiates from standard wireless communications with its dramatically higher and varying propagation delays [14], even up to hours [5], 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 this section, a new diffusion-based model for molecular communication, whose main distinction with respect to previously proposed models, such as [9] and [6], 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 [28].

We analyze the stochastic nature of a basic point-to-point messenger-based molecular communication model with one nano-transmitter and one nano-receiver, 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.

1.2.2 Molecular Channel Model with Multiple Bit Carrying Molecules

Existing diffusion-based molecular communication models encode information on the concentration of the molecules [55, 54]. In this chapter, effects of information encoding on multiple atoms of the messenger molecule on channel capacity are studied. We introduce a messenger-based molecular communication model, in which information is encoded on the atoms of polyethylene molecules which are in the form of $CH_3(CHX)_nCH_2F$, where X is either an H or F atom, representing a 0 and a 1 bit, respectively. Encoded molecules are assumed to be released into the medium by sender nanomachines and left to propagate following a Brownian Motion process to the receiver nanomachine. Then, the capacity of this channel is derived and the parameters optimizing it are assessed.

Using an erasure channel model, we derived the parameters affecting the capacity which are molecule size, number of redundant molecules for one transmission and molecule lifetime. We derived an expression for the optimal number bits maximizing the capacity.

1.2.3 Forward Error Correction for Molecular Nanonetworks

Existing works on molecular communication concentrates especially on channel modelling for capacity and noise analysis for molecular communication by diffusion [6, 9, 19, 55, 57]. However few of them deal with error compensation [58, 59, 60]. Nevertheless, because of the stochastic nature of molecule propagation by Brownian Motion, a thorough analysis of error compensation is needed. In this sense, Forward Error Correction (FEC) is proposed as a promising solution appropriate for the molecular communication environment since it does not require a reverse channel from the receiver to the transmitter which is required for other error correction mechanisms such as Automatic Repeat Request (ARQ) which costs production and transmission of new molecules representing the acknowledgements.

1.3 Thesis Outline

This thesis is organized as follows: In Chapter 2, we propose a novel communication model for molecular communication by diffusion where information is encoded on the atoms of polyethylene molecules in the form $CH_3(CHX)_nCH_2F$, where X is replaced by H and F atoms representing 0 and 1 bits, respectively. The main processes of the proposed communication model are introduced. Then the rate-delay of tradeoff of the system is investigated and network coding technique is proposed to improve this tradeoff. In Chapter 3, the same communication model introduced in Chapter 2 is used with modifications to fit a use case scenario where the polyethylene molecules

are utilized for transferring information in blood through human body. The channel model for human body environment is built and its capacity is investigated for varying parameters. A numerical analysis is conducted to find a closed form expression for the optimal number of bits maximizing the capacity in terms of molecule lifetime and number of released molecules for one transmission. In Chapter 4, using the same communication model, we investigated using forward error correction for ameliorating the system performance. The improvement in bit error rate by using simple linear block codes is illustrated. In Chapter 6, we conclude the thesis by summarizing the contribution of this thesis and underlining future research challenges.

Chapter 2

RATE-DELAY TRADEOFF WITH NETWORK CODING IN MOLECULAR NANONETWORKS

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 chapter, first, a new messenger-based molecular communication model, which includes a nano-transmitter sending information to a nano-receiver, 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.

2.1 Introduction

Advances in nano and biotechnology require the development of biocompatible nanomachines, which have fundamental roles in complex bio-hybrid 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, organs. In order to attain macro scale 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, nano-processors and nano-memory, and medical applications, which are drug delivery, disease treatment and health monitoring [1].

Despite the novelty of molecular commmunication, there several physical implementations such as [15] where Cu^{2+} ions are used as information carrying molecules. With the help of fluorescence microscopic observations, in [16], the hybridization of DNA is used to employ a molecular communication path between vesicles. A physical reception mechanism is discussed in [17] where a biomimetic nanosensory device is implemented for detection and amplification of biologically important entities.

In the literature, the studies are concentrated on modelling [6], capacity [9], [18], noise analysis of molecular channels [19], 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], [24].

Molecular communication differentiates from standard wireless communications with its dramatically higher and varying propagation delays [14], even up to hours [5], 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 electro-magnetic networks with composite links [25], to optimize rate for two-layered, namely, physical and network packet transmission system [26], and mitigate delay in multipath routed and network coded networks [27]. Albeit these studies point out the rate-delay tradeoffs for classical communication domains, no study has concentrated on the trade-off between rate and delay in molecular communications, which led us to this very study.

In this study, a new diffusion-based model for molecular communication, whose main distinction with respect to previously proposed models, such as [9] and [6], 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 [28].

We analyze the stochastic nature of a basic point-to-point messenger-based molecular communication model with one nano-transmitter and one nano-receiver, 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 2.4.

The remainder of this chapter is organized as follows. Using the messenger-based molecular communication model introduced in Section 2.2, we investigate the delay characteristics of this model. In Section 2.3, 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 2.2 and 2.3 are evaluated numerically and the results on the rate-delay tradeoff are discussed thoroughly in Section 2.4.

2.2 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 [45]. 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 [45]. 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 study, a messenger-based molecular communication model is proposed. This model includes partially fluorinated polyethylene messenger molecules, $CH_3(CHX)_nCH_2F$, 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 [5]. 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 travelled by the messenger molecule [5].

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

2.2.1 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 nano-receptors such as molecular pumps or sorting rotors due to the special structure of these molecules containing a distinctive head [5].

The partially fluorinated polyethylene molecule [5] 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 $\sim 1\ bit/nm^3$ [5], which is widely suggested as an information storing molecule. Suggested in [50] for nanocomputer memory systems, a partially fluorinated polyethylene molecule is in the form $CH_3(CHX)_nCH_2F$, 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 nano-transmitter. 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 [5]. $n \neq l_m$ 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, CH_3 and CH_2F forming the two ends of the molecule, provides a decoding order for the message.

To increase the information carrying capacity of messengers, one needs larger molecules. However, larger molecules diffuse more slowly. According to the Einstein-Stokes relation [53], the diffusion coefficient D is inversely related with the size of the particles, i.e., $D = k_BT/6\pi\eta r$, where k_B is Boltzmann's constant, T is the absolute

temperature and η is viscosity.

The information encoding process described here can exploit a molecular modulation technique such as Molecule Shift Keying (MoSK) introduced in [23]. 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 [23], a $n = 2$ bit constellation diagram for Quadruple MoSK realized by fluorinated polyethylene is shown in Fig. 4.1.

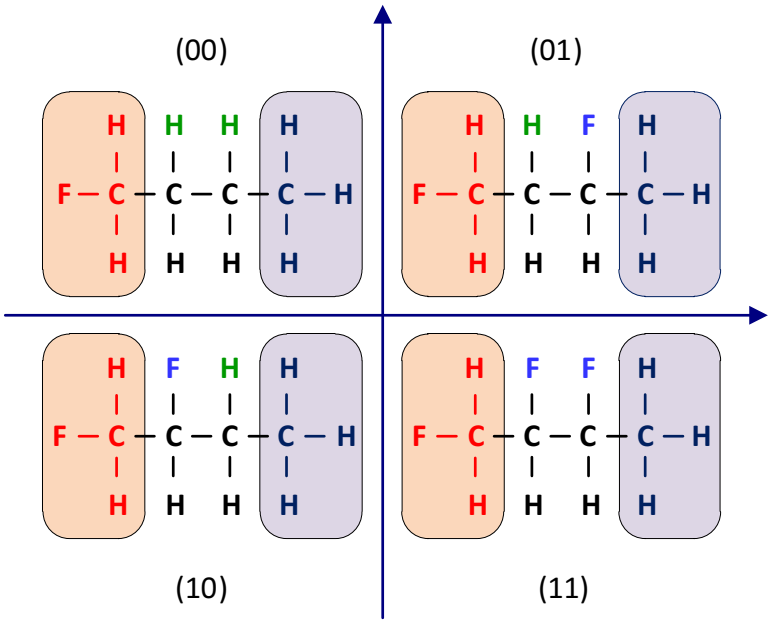

Figure 2.1: Constellation diagram for QMoSK modulation, $n = 2$.

2.2.2 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 release 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 [31] as in the case of insect pheromone release [32], [33] . 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

$$R^{(TX)} = \frac{l_m}{N_P T_M}, \tag{2.1}$$

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

2.2.3 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 [20], i.e.,

$$f_\tau(\tau) = \frac{d}{\sqrt{4\pi D\tau^3}} \exp\left(-\frac{(\nu\tau - d)^2}{4D\tau}\right), \ \ \tau \geq 0, \tag{2.2}$$

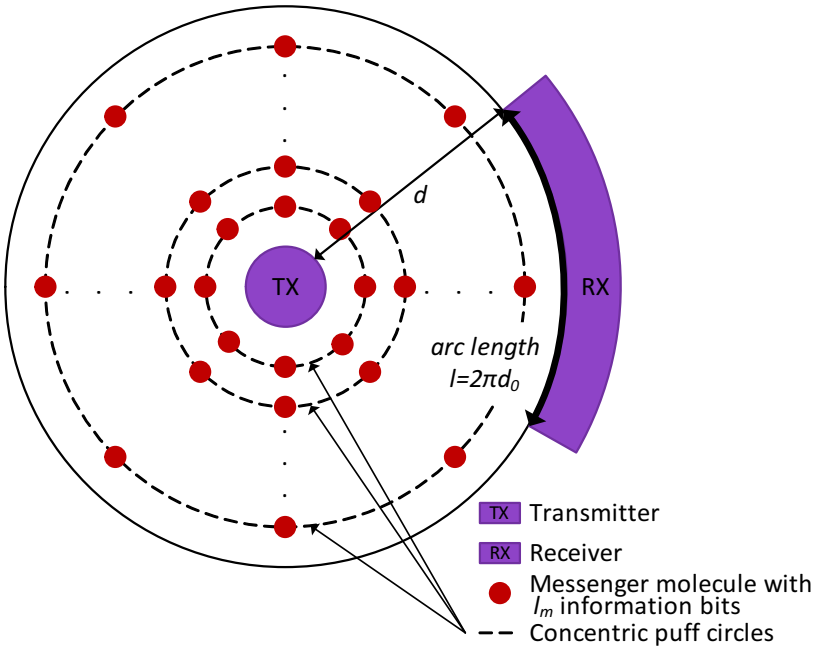

Figure 2.2: Particle propagation and detection processes.

where v is the mean drift velocity of the medium, 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.

2.2.4 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

$$R^{(RX)} = \frac{l_m}{N_P T_M}. \tag{2.3}$$

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 i^{th} 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 i^{th} 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 by

$$P_M(t) = 1 - \prod_{i=1}^{N_P} [1 - F_\tau(t - iT_M)]^{N_M}, \tag{2.4}$$

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

$$P_d = \begin{cases} 1, & \text{if } d \leq d_0 \\ \frac{d_0}{d}, & \text{if } d > d_0 \end{cases} . \tag{2.5}$$

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. 3.2. 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 non-received message. The probability $P_M(t)$ in (2.4) can be modified as a conditional probability, where M is the event that the message is received, i.e.,

$$P_M(t|\mathrm{M}) = \frac{1 - \prod_{i=1}^{N_P} \left[1 - P_d F_\tau(t - iT_M)\right]^{N_M}}{P_r}. \tag{2.6}$$

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,

$$E\left\{\tau_M|\mathrm{M}\right\} = \int_0^\infty \left(1 - F_{\tau_M}(t)\right) dt. \tag{2.7}$$

For a single puff containing a single molecule, i.e., $N_M = 1$ and $N_P = 1$ in (2.6), the CDF of the delay, $F_{\tau_M}(t)$, becomes equal to $F_\tau(t)$ whose pdf is given in (2.2). Hence, the expected message propagation delay is equal to d/ν, the expected value of $F_\tau(t)$.

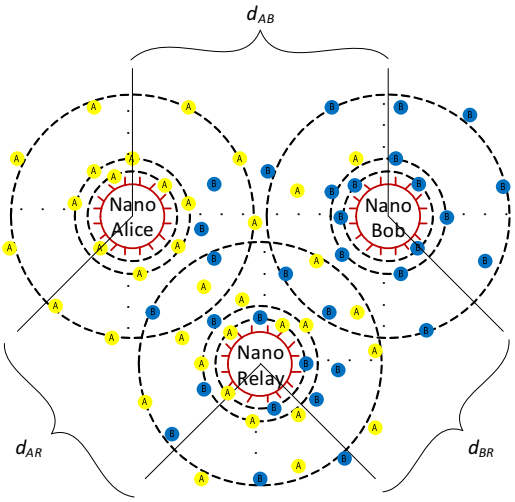

Figure 2.3: A simple uncoded network mechanism.

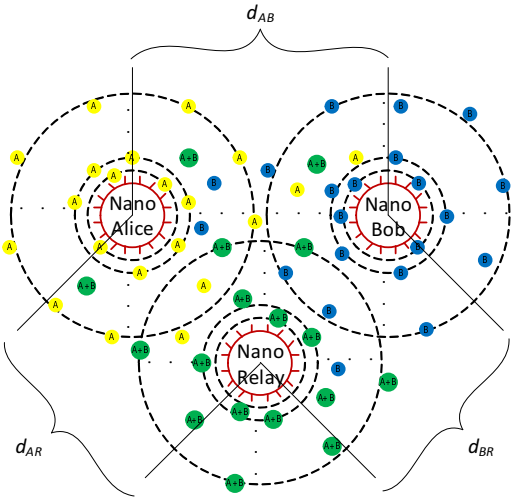

Figure 2.4: A simple network coding mechanism.

2.2.5 Information Decoding Process

Decoding of the messages is realized as the demodulation of the incoming molecule stream according to MoSK described in Section 4.2.1. 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 [34] 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 [35]. 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 4.2.1 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 2.2.2. To reduce the energy for decoding the redundant molecules, the receiver waits during $T_{wait} = \alpha N_P T_M$ ($\alpha > 1$), after the reception of the first message since a second one cannot be generated by the transmitter in a time duration of $N_P T_M$.

2.3 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. 2.3, where Nano-Alice and Nano-Bob need to send each other a message.

Nano-Alice and Nano-Bob function as both nano-transmitter and nano-receiver realizing all the five main processes mentioned in Section 2.2. Assume that Nano-Alice and Nano-Bob are not 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 nano-transmitter and a nano-receiver. 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 [43]. 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.

2.3.1 Rate-Delay Tradeoff for 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

$$E\{T_D\} = E\{T_D|AB\}\, P(AB) + E\left\{T_D|\overline{AB}\right\} P(\overline{AB}), \tag{2.8}$$

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 $E\left\{T_D|\overline{AB}\right\} = E\left\{T_{ARB}\right\}$, 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, $E\left\{T_D|AB\right\} = E\left\{\min(T_{AB}, T_{ARB})\right\}$, where T_{AB} is the delay for the path AB.

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

$$E\left\{T_D|AB\right\} < E\left\{T_{AB}\right\} = E\left\{\tau_M\right\}. \tag{2.9}$$

Then, the expected message delay between A and B using (2.7) is

$$E\{\tau_M\} = \int_0^\infty \left[\frac{\prod_{i=1}^{N_P}\left(1 - P_d F_\tau\left(t - iT_M\right)\right)^{N_M} - \left(1 - P_d\right)^{N_P N_M}}{1 - \left(1 - P_d\right)^{N_P N_M}}\right] dt. \tag{2.10}$$

Nevertheless, it is troublesome to find a closed-form expression using (2.10). 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

$$E\left\{\tau_M\right\} > \frac{1 - \left(1 - P_d\right)^{N_P N_M + 1} - P_d\left(N_P N_M + 1\right)\left(1 - P_d\right)^{N_P N_M}}{\xi P_d\left(N_P N_M + 1\right) P_r}. \tag{2.11}$$

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

$$F_{\tau^{(u)}}(t) = \begin{cases} t/\xi, & \text{if } t \in (0, \xi) \\ 1, & \text{if } t \geq \xi \\ 0, & \text{else} \end{cases}, \tag{2.12}$$

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., $\xi = (-3D +$

$\sqrt{9D^2+d^2v^2})/v^2 > 0$. 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 (2.11) calculated by substituting (2.12) into $F_\tau\left(t - iT_M\right)$ for each i in (2.10).

Similar to lower bound in (2.11), an upper bound is obtained as

$$\begin{aligned} E\left\{\tau_M\right\} < & -\frac{\left(1-P_d\right)^{N_P N_M}}{P_r} \\ & + \frac{\left(1-P_d N_P N_M/\mu\right)^{N_P N_M+1} - \left(1-P_d(N_P N_M+\mu)/\mu\right)^{N_P N_M+1}}{\mu P_d\left(N_P N_M+1\right) P_r}. \end{aligned} \tag{2.13}$$

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

$$F_{\tau^{(v)}}(t) = \begin{cases} t/\mu, & \text{if } t \in (0, \mu) \\ 1, & \text{if } t \geq \mu \\ 0, & \text{else} \end{cases}, \tag{2.14}$$

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 (2.10), 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 (2.13). Using (2.9), we obtain

$$E\{T_D\} < E\{T_{AB}\}P(AB) + \left(E\{T_{ARB}\} + E\{T_q\}\right)P(\overline{AB}). \tag{2.15}$$

$E\left\{T_q\right\}$ is included in (2.15) to represent the expected queuing delay for message A in the Nano-Relay defined in Section 2.3.1.

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, $E\left\{{T_q}^{(\overline{C})}\right\}$, which is expressed by $E\left\{{T_q}^{(\overline{C})}\right\} = P\left\{Q^{(\overline{C})}\right\} E\left\{{T_q}^{(\overline{C})}|Q^{(\overline{C})}\right\}$, where $Q^{(\overline{C})}$ is the event that A is received in the transmission period of B. The probability of queueing in uncoded case is

$$P\left\{Q^{(\overline{C})}\right\} = Pr\left\{N_P T_M > \tau_A - \tau_B > 0\right\}, \tag{2.16}$$

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 $P\left\{Q^{(\overline{C})}\right\}$ is given by

$$P\left\{Q^{(\overline{C})}\right\} = \frac{d_{AR}}{d_{AR}+d_{BR}}\left(1-\exp\left(-\frac{\nu N_P^2 T_M}{d_{AR}}\right)\right). \tag{2.17}$$

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* [38]. 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 [38] as

$$E\left\{T_q|Q^{(\overline{C})}\right\} = \frac{1}{2}\frac{(\alpha+\beta)N_P^2 T_M^2}{1-(\alpha+\beta)N_P T_M}. \tag{2.18}$$

Similar to the reception rate calculation in 2.2.4, reception rate of Nano-Alice's messages at Nano-Bob can be calculated as

$$R_{\overline{C}}^{(RX)} = \frac{l_m}{N_P T_M}. \tag{2.19}$$

2.3.2 Rate-Delay Tradeoff for Network Coded Case

Now, consider the case when Nano-Relay uses a network coding mechanism, which is shown in Fig. 2.4. When Nano-Relay receives a message, it starts waiting T_W seconds for the other message to arrive before transmitting the received message. If the other message arrives within T_W seconds, 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

$$E\left\{T_q^{(C)}\right\} = P\left\{W^{(C)}\right\} E\left\{T_q^{(C)}|W\right\} + P\left\{\overline{W}^{(C)}\right\} T_W, \tag{2.20}$$

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

$$P\left\{W^{(C)}\right\} = \frac{d_{BR}}{d_{BR}+d_{BR}}\left(1-\exp\left(-\frac{\nu N_P T_W}{d_{BR}}\right)\right). \tag{2.21}$$

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 network coded case can be calculated by

$$E\left\{T_q^{(C)}|W\right\} = \frac{(1-0.75P_{AXB})(\alpha+\beta)N_P^2 T_M^2}{2\left(1-(\alpha+\beta)(1-0.5P_{AXB})N_P T_M\right)}, \tag{2.22}$$

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 2.2.4, reception rate of Nano-Alice's messages at Nano-Bob can be calculated as

$$R_C^{(RX)} = \frac{l_m}{N_P T_M}\left(2P\left\{W^C\right\} + \left(1 - P\left\{W^C\right\}\right)\right). \tag{2.23}$$

2.4 Simulations

In this section, we evaluate rate and delay expressions found in Section 2.2 & 2.3 with the simulation parameters given in Table 2.1, chosen in agreement with [5]. Then, the uncoded and the network coded cases are compared to reveal the rate-delay tradeoff.

2.4.1 Simulation for Uncoded Case

We investigate the rate-delay tradeoff of the uncoded case without a relay in Fig. 2.5 to illustrate the decaying trend of rate and delay with increasing N_P. The rate expression in (2.3) is utilized to evaluate the rate variation. Our analysis is not based

Table 2.1: 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

on the exact expressions of the delay but on the lower and upper bounds, given in (2.11) and (2.13). Although the two bounds follow the same trend, the lower bound is far beyond the realistic propagation delays in molecular domain, hence, upper bound (2.13) 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 are

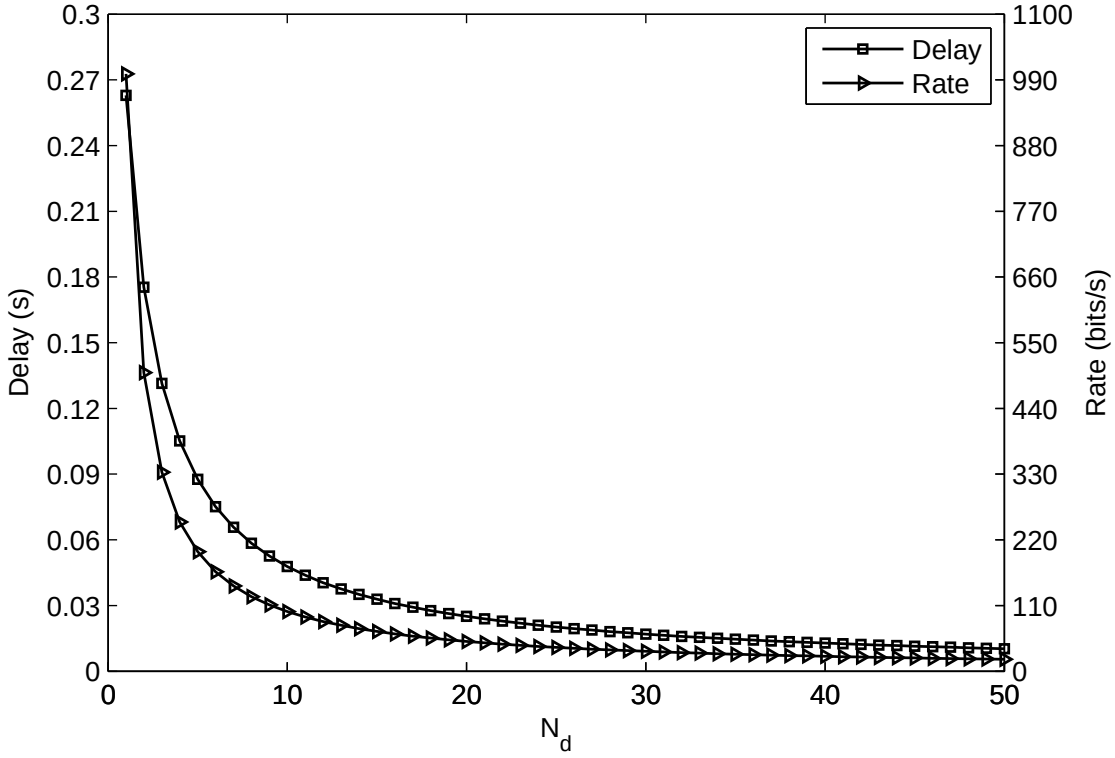

Figure 2.5: Delay and rate characteristics with N_P.

also intuitively expected from (2.3), (2.11) and (2.13). The tradeoff between rate and delay is illustrated in Fig. 2.6. 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 [36] 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 [37]. 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

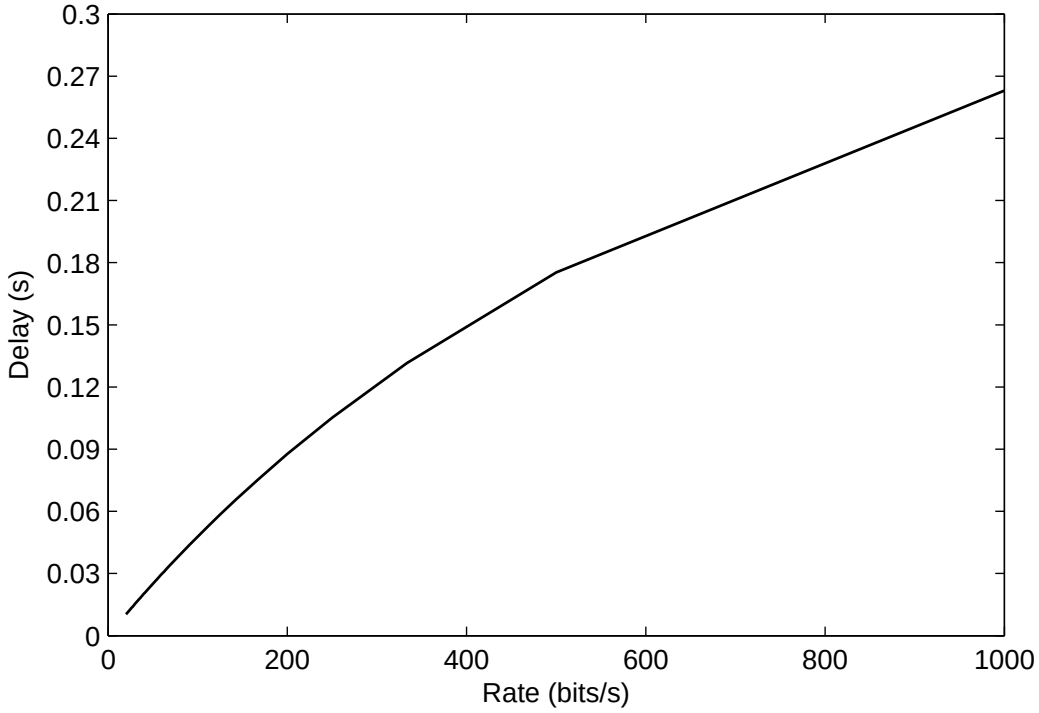

Figure 2.6: Rate vs delay analysis.

DNA computations are highly investigated in various studies such as [39] and [40].

2.4.2 Simulation for Network Coded Case

In Fig. 2.7, 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

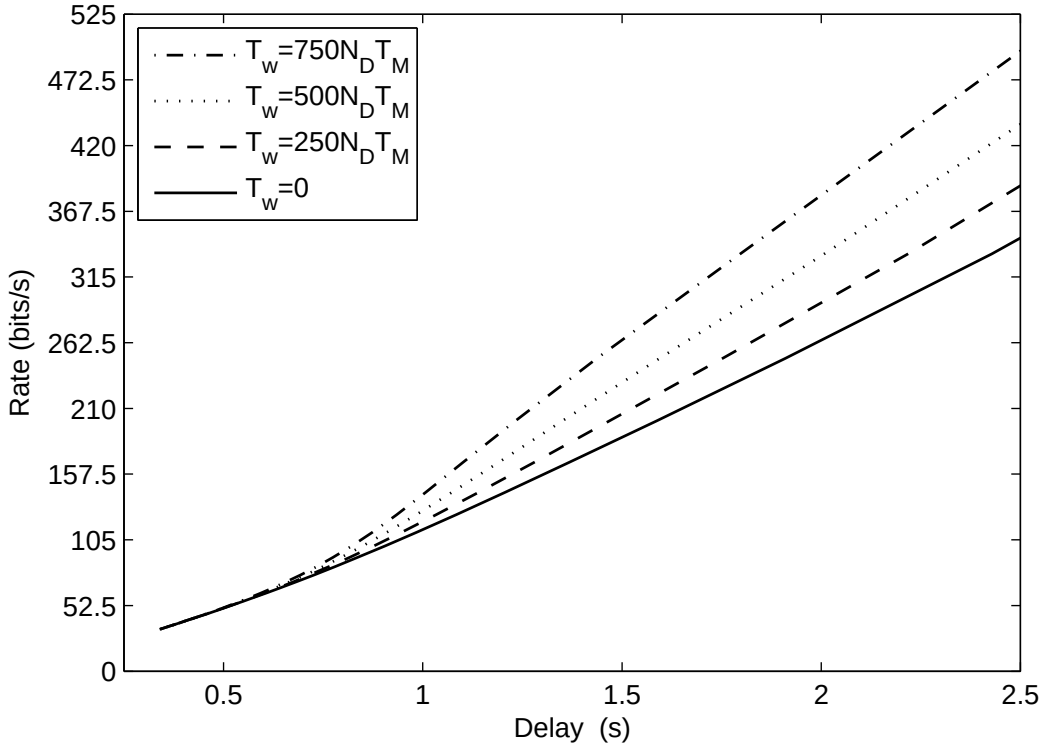

Figure 2.7: Rate vs delay analysis in uncoded and coded network cases.

messages to decrease the number of transmitted messages. As illustrated in Fig. 2.7, by increasing the waiting time T_W, 40% higher reception rate compared to 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 [41], 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 behaviours of engineered

bacteria used in cancer therapy [42]. 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.

Chapter 3

MOLECULAR CHANNEL MODEL WITH MULTIPLE BIT CARRYING MOLECULES

Molecular communication is a bio-inspired paradigm, proposed to communicate nanomachines via diffusion of molecules through an aqueous medium. The type and structure of the molecules to be propagated bear great importance since they directly affect the modulation structure of molecular communication. We propose a messenger-based molecular communication model where information is encoded on the atoms of polyethylene molecules in the form of $CH_3(CHX)_nCH_2F$, where X is either an H or F atom, representing 0 and 1 bits, respectively. The encoded polyethylene molecules are released from the transmitter nanomachine, and their propagation towards the receiver is modelled as a Brownian Motion. Using an erasure channel model, our analysis focuses on calculating the capacity of this channel and revealing the parameters affecting it such as molecule size and number of redundant molecules for one transmission.

3.1 Introduction

Molecular communication is a new bio-inspired paradigm. Biological phenomena, such as inter-cellular communications by the transport of vesicles and hormones enabling inter-organ communications have recently inspired the communications by the dispatch, propagation and reception of molecules in the context of nanomachines. Nanomachines are nanoscale devices, and can be naturally existent (i.e. biological

cells) or artificially synthesized (i.e. bioengineered cells) [55]. Molecular communication allows nanomachines to encode outgoing information to molecules, to let messenger molecules propagate in an aqueous medium and to decode information from incoming molecules. Molecular communication is very suitable for nanomachines not only because of its low complexity and low energy requirements but also for its ability to network simple nanomachines to coordinate and carry out complex tasks. Potential application areas of networked nanomachines by molecular communication include but are not limited to medicine, monitoring, quality control and attack detection.

Existing diffusion-based molecular communication models encode information on the concentration of the molecules [55, 54]. In this study, effects of information encoding on multiple atoms of the messenger molecule on channel capacity are studied. We introduce a messenger-based molecular communication model, in which information is encoded on the atoms of polyethylene molecules which are in the form of $CH_3(CHX)_nCH_2F$, where X is either an H or F atom, representing a 0 and a 1 bit, respectively. Encoded molecules are assumed to be released into the medium by sender nanomachines and left to propagate following a Brownian Motion process to the receiver nanomachine. Then, the capacity of this channel is derived and the parameters optimizing it are assessed. Novelty of our work can be summarized as follows:

- Multiple bits are assumed to be encoded on a single polyethylene molecule, and are communicated between two nanomachines in a single propagation session.

- Multiple bit encoding on single messenger molecule corresponds to data link layer packets in traditional networking, since it can include the transmitter and receiver identifications and sequence numbers. This fact allows us to move one

step forward from physical layer to the data link layer in molecular communications.

- Multiple bit carrying molecules bypass the need for synchronization among nanomachines, by including data packet sequence numbers.

- Results reveal the conditions for which multiple bit carrying molecules is a viable method for molecular communications, for a use case scenario.

The remainder of this chapter is organized as follows. In Section 4.2, the molecular communication model with multiple bit carrying molecules is introduced. The channel model and the capacity calculation are given in Section 4.3. The numerical results on the capacity and the effects of the communication channel parameters on it are provided in Section 3.4.

3.2 Molecular Communication Model

The messenger molecule considered for this model is partially fluorinated polyethylene, i.e., $CH_3(CHX)_nCH_2F$, carrying n bits of information via diffusion in the communication medium. The predefined atom X is replaced by an Hydrogen (H) or Fluorine (F) atom to represent the bit 0 or the bit 1. Some forms of these fluorinated polythylene molecules are utilized as oxygen carriers in artificial blood formulations [51]. In our model, we focus on these molecules called fluorinated hydrocarbon perfusants and assume that they propagate in human blood as a use case.

The value of n in the molecule's formula can reach up to 10^9 bits [5], thus by the reception of such a single polyethylene molecule, 10^9 bits of information can be transferred. However, because of the slow diffusion of large molecules, propagation delays definitely rise. Thus, it is important to find find an optimum value for molecule size in the capacity sense.

In our model, transmitters are considered as nanomachines capable of producing polyethylene molecules on which the information is encoded and emitting them into the fluid medium. Receivers are nanomachines with specific receptors capable of capturing polyethylene molecules arriving to its affinity and decoding the information encoded on these molecules. These nanomachines are considered to be in a fluid medium where the messenger molecules propagate by Brownian motion.

Our model embodies five main processes; namely; information encoding process, transmission process, propagation process, reception process and information decoding process.

3.2.1 Information Encoding Process

In this model, the transmitter (TX) nanomachine generates messenger molecules carrying n bits of information. Firstly, an ideal messenger molecule should be easily recognized by nano receptors due to the special structure of these molecules containing a distinctive head and tail. Secondly, these molecules should be bioinactive, not easily corrupted by natural processes before they reach the receiver (RX) nanomachine [5].

Partially fluorinated polyethylene molecules are candidates for such messenger molecules as suggested in [50]. A partially fluorinated polyethylene molecule is in the form $CH_3(CHX)_nCH_2F$, where X is either an H or F atom, representing the 0 and 1 bits, respectively. CH_3 and CH_2F form the distinctive head and tail of the molecule, providing a decoding order for the receiver. Hence, headers that are assured to be read first, may be added to the front of the data which may be used to store TX and RX identifiers, parity and checksum bits, flags that are needed to step up from the physical layer to data link layer. This structure enables the knowledge transfer from classical wireless communications techniques to molecular communication for some

concepts such as routing, medium access control, reliability.

Furthermore, the carbon chain of polyethylene is assumed to contain the encoded atoms only in one side of the chain for the sake of readibility and the other side is assumed to be full of H atoms. We assume also that an encoded polyethylene carries 50% H and 50% F atoms on the average on the coded side of the molecule to have equal diffusion coefficients for each encoded molecule. According to these assumptions, the information density of this molecule is $d_{message} \sim 26\ bits/nm^3$, a significantly higher number compared to a more common molecule, DNA, whose information density is $\sim 1\ bit/nm^3$ [5] which leads us to prefer fluorinated polyethylene to DNA.

The information capacity of a single molecule increases with increasing n, in exchange for a larger molecule size which slows down the diffusion of the molecule. The diffusion coefficient for spherical particles through liquid is expressed by the Einstein-Stokes equation [53] as $D = k_B T/6\pi\eta r$, where k_B is the Boltzmann's constant, T is the absolute temperature, η is viscosity and r is the radius of the nanomachine [53].

Molecule Shift Keying (MoSK), a molecular modulation technique introduced in [23], can be exploited for the information encoding process of this study. This modulation scheme requires 2^n different molecules to represent n bits of logical information. For the transmission of an intended symbol, one of these molecules is released by the transmitter and the receiver decodes the intended symbol according to the type of the received molecule. An example $n = 2$ bit constellation diagram for Quadruple MoSK is shown in Fig. 4.1 [23]. In our case, n can reach up to the order of 10^4 and corresponding constellation diagrams are similar to the diagram in Fig. 4.1.

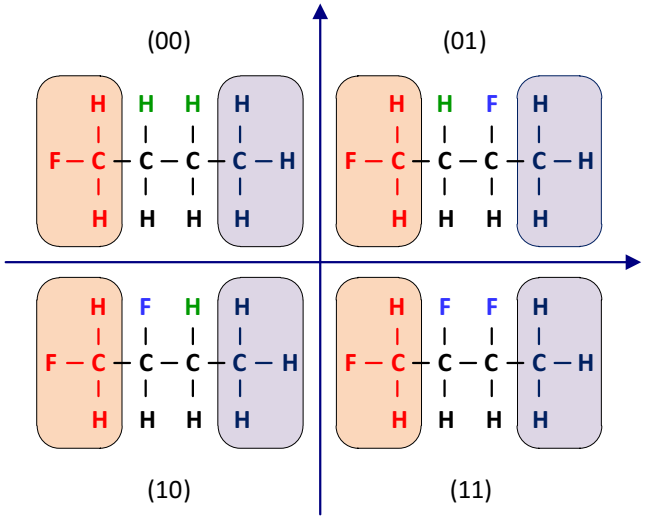

Figure 3.1: Constellation diagram for QMoSK modulation, $n = 2$ [23].

3.2.2 Transmission Process

The TX nanomachine is assumed to have a spherical shape and the messenger molecules are released to the medium from the boundary of the nanomachine. This emission process is uniformly distributed over this spherical boundary, called the emission boundary as seen in Fig. 3.2. Since the messenger molecules are assumed to propagate by Brownian Motion in the medium in all directions, the probability that a single molecule reaches the receiver in a given time is very small. Besides, the messenger molecules can be degraded by the environment. Hence, for the sake of reliability, the transmitter emits redundant copies of the molecule, namely N_M copies, for each message in order to raise the reception probability. The booster effect on channel capacity of using extra molecules where the information is encoded in the concentration of the molecules is illustrated in [55]. In this study, we use the same method to boost the channel capacity where the information is encoded in the type of the molecule.

Emission of the molecules takes place instantaneously which is inspired from the

emission of pheromones in animals in alarming situations such as threats from predators, injured conspecifics, and exposure to toxic compounds [31].

3.2.3 Propagation Process

Messenger molecules released from the transmitter propagate in the fluid medium by diffusion. The random motion of the messenger molecules is modelled as Brownian. We assume that the total concentration of emitted molecules are much lower than the concentration of all fluid molecules. Therefore, the interactions between molecules are neglected and the movement of each molecule is assumed independent. Considering these assumptions, we can express the concentration of the molecules by Fick's law of diffusion [54]. For instantaneous emission of the messenger molecules described in Section 4.2.2, the first hitting time t of an emitted molecule to a spherical surface at a distance d from the emission boundary is distributed as an inverse Gaussian pdf [55], i.e.,

$$f(t) = \frac{d}{\sqrt{4\pi D t^3}} \exp\left(\frac{-d^2}{4Dt}\right), \quad t \geq 0, \tag{3.1}$$

where D is the diffusion coefficient.

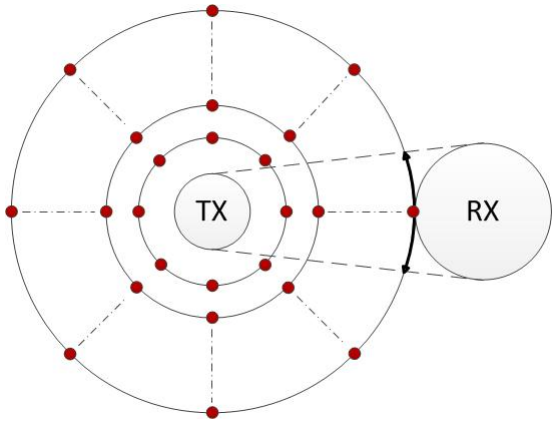

Figure 3.2: Particle propagation and detection processes.

3.2.4 Reception Process

RX nanomachine has specific receptors which bind to the messenger molecules arriving to their vicinity. When a messenger molecule hits the boundary of the receiver, it is assumed to be instantly captured for decoding.

We assume that reception of only one of the N_M molecules released for a single message is sufficient for decoding the message. Thus, we need a mechanism to recognize the extra molecules arriving to the receiver after the reception of the first molecule carrying the same information. Besides, residual molecules from the previous messages may arrive to the receiver during the reception of the current message and may be misinterpreted as the current message. To cope with these two problems, the transmitter adds extra message identifier bits to the regular information bits such that the receiver can identify to which message that the incoming molecule belongs and does not decode the molecules arriving to the receiver after the reception of the first molecule with the same identifier.

3.2.5 Decoding Process

By exploiting the special structure of the molecule described in Section 4.2.2, the receiver reads the information encoded on the incoming molecules, right after reception. The head and tail structure enables the receiver to know from which end of the molecule it should start decoding. Furthermore, since only one side of the molecule is encoded, the receiver also knows which side should be decoded. The molecule captured by the receiver is decoded by the demodulation of the incoming molecule generated according to MoSK presented in Section 4.2.2. An alternative decoding scheme is reading the molecule bit by bit. The difference in interaction energies between the coded H and F atoms and the boron atom, B, of a C_5H_5B or $C_3H_3N_2B$ probe reveals the type of the coded atom [35].

3.3 Channel Model

Using the communication model proposed in Section 4.2, we put forward a channel model between a TX and a RX nanomachine for the messenger based molecular communication.

The message-carrying fluorinated polyethylene molecules are generally biocompatible, even though a thorough study for toxicity levels of different types of polyethylene molecules is still required [5]. Some of the fluorinated polyethylene molecules are FDA approved to be used in artificial blood formulations [51]. Thus we consider that the proposed communication model operates in human body transferring information by polyethylene molecules propagating in blood.

In this model, transmitter emits multiple molecules of each message for reliability. When one of the emitted molecules reaches the receiver, information transmission is considered to be successful. Otherwise, when none reach the receiver, the transmission is considered erroneous. Although polyethylene molecules are considered stable and chemically inert [51], they are cleared from blood by the immune system. Monocytes or macrophages ingest these molecules and clear them rapidly from the blood [52]. For successful reception of a messenger molecule, it has to reach the RX nanomachine before being caught by the immune system. The environment does not damage the bit information carried on H and F atoms since the fluorinated polyethylene molecules are proven to be chemically inert [51]. If one molecule reaches the receiver, it completely yields the message without any bit error. Otherwise, when none of the messenger molecule copies arrive to the receiver due to random motion or phagocytosis, information carried by these messenger molecules is assumed to be erased. In this case, the communication is modelled by a block erasure channel, illustrated in Fig. 3.3, where each block of n bits are either jointly received with probability $(1-\alpha)$ or jointly erased with probability α. The information sent over the molecular channel is

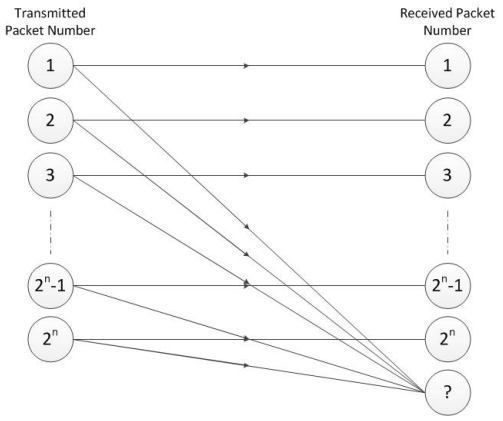

Figure 3.3: Block erasure channel.

$X^n \in \{0,1\}^n$ and the information received is $Y^n \in \{0,1\}^n$ if the block is not erased in the channel.

This channel model does not require synchronisation, since the messenger molecules carry not only data bits but also identification bits. From the sequence numbers, erased messages by the channel can be recognized by the RX nanomachine.

To find the probability of erasure α, it is assumed that messenger molecules are cleared from blood at an exponential rate λ [51]. Then, a released polyethylene molecule has a lifetime $\tau = 1/\lambda$, after which it is considered to be cleared from blood. q, probability that a molecule reaches the receiver in τ seconds, before lifetime of the molecule, is given by

$$q = \int_0^\tau f(t)dt \tag{3.2}$$

where $f(t)$ is the probability density function of first hitting time of a molecule to the receiver, given in (4.3). Then, the probability of erasure, α which is the probability that none of the N_M molecules belonging to the same message arrive to the receiver is expressed by

$$\alpha = (1-q)^{N_M}. \tag{3.3}$$

Knowing the block erasure probability α, the capacity of this channel can be calculated as

$$C_e = (1 - \alpha)n. \tag{3.4}$$

By inserting (4.4) and (3.3) into (3.4), the capacity expression is

$$C_e = \left(1 - \left(1 - \int_0^{\tau} f(t)dt\right)^{N_M}\right) n \text{ bits/channel use.} \tag{3.5}$$

Clearly, capacity of the molecular channel depends on the lifetime of the polyethylene molecule in the blood τ, the number of redundant molecules N_M, the diffusion coefficient D, the distance between the transmitter and the receiver d and the number of bits encoded onto a molecule n.

While the effects of N_M, τ and d on the erasure channel capacity is straightforward, the effect of a change in n is not clear. Increasing n seems to allow higher capacity when D, the diffusion coefficient of the molecules is fixed. However, when n increases, it means that more atoms are added in the polyethylene molecule which makes it larger. The larger molecule size decreases the diffusion coefficient, D, thus the diffusion speed of the molecules. Hence, the number of molecules able to reach the receiver before τ lowers which have a negative influence on the capacity. Therefore, it is handy to find n which maximizes the capacity for the erasure channel.

3.4 Numerical Results

In this section, we assess the effects of numerous communication parameters on molecular erasure channel capacity.

3.4.1 Effect of Molecule Size

Here, we consider the effect of varying n on the polyethylene molecule formula $CH_3(CHX)_nCH_2F$. The effect of n on the successful reception of the molecule within

its τ lifetime is not trivial. Fig. 3.4 assesses the achievable erasure channel capacity for varying n. For this assessment, the lifetime τ is fixed to 100 seconds which is an approximate value for the lifetime of fluorinated polyethylene in the human intravascular system for artificial blood applications [52], and TX-RX distance is assumed 50 μm [5]. Human blood has a viscosity in the range 20×10^{-3} to $40 \times 10^{-3} kg/m-s$ [5].

In Fig. 3.4, erasure channel capacities for different medium viscosity levels are presented. Clearly, the viscosity of the medium has a great impact on the optimal alphabet size for capacity. As expected, with increasing viscosity, optimal n values that achieve maximum channel capacity decrease.

3.4.2 Effect of Lifetime τ

Since the messenger molecules move randomly in the propagation medium, not all the N_M molecules emitted for a message reach the receiver. To improve the probability of reception, synthesizing molecules with longer lifetime against phagocytes is considered. In Fig. 3.5, the capacity of the proposed molecular channel is evaluated with respect to varying n for different lifetimes. The viscosity of the medium is fixed to 30×10^{-3} $kg/m-s$ and the number of emitted molecules is fixed to 1000. As seen Fig. 3.5, an increase in τ significantly improves the capacity. Thus, to find the optimal n, the lifetime τ should also be considered as a significant parameter.

3.4.3 Effect of Number of Redundant Molecules N_M

Because of the random motion of messenger molecules, successful reception cannot be guaranteed. To increase the probability of reception, redundant identical molecules are used. N_M identical copies of the messenger molecule are released. In Fig. 3.6, it is clearly seen that as the number of redundant molecules is higher, the capacity

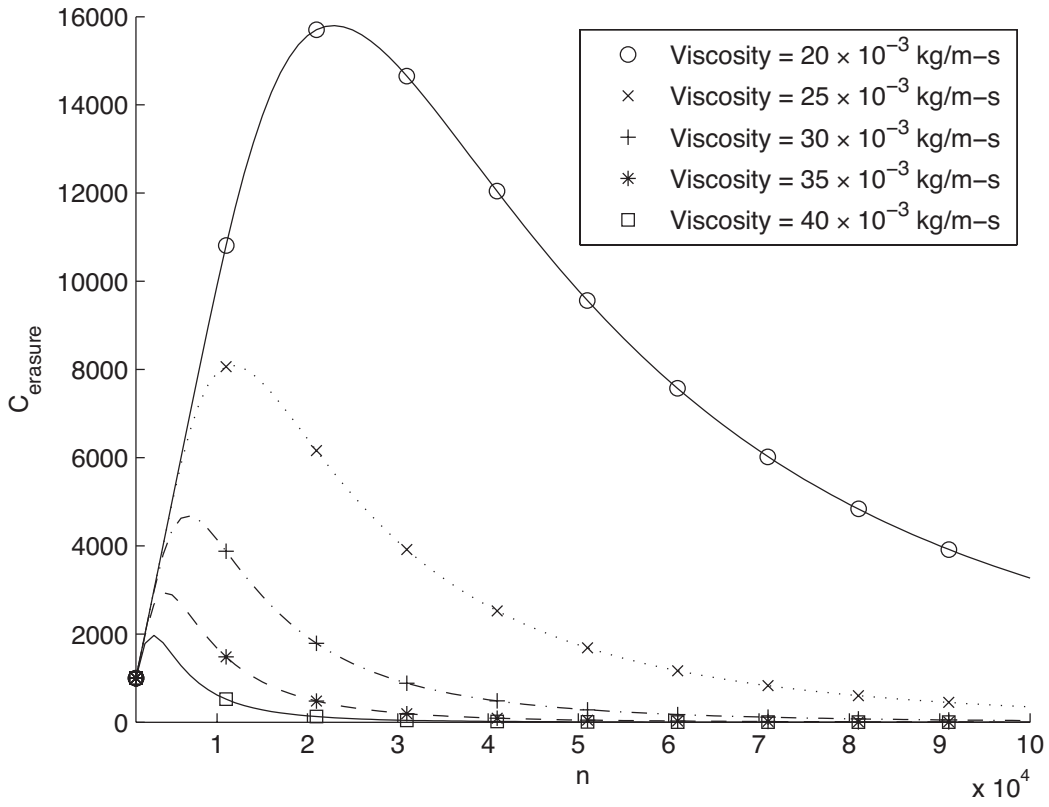

Figure 3.4: Capacity of molecular erasure channel for varying n (i.e., molecular size) with different viscosities

becomes higher since the probability of reception of the message is increased.

3.4.4 Optimal Number of Bits In a Molecule n

For the fluorinated polyethylene, Fig. 3.4,3.5 and 3.6 illustrate that the number of bits encoded on a molecule, n, which maximizes the capacity, changes with changing molecule lifetime, τ and number of redundant molecules, N_M. An analytical solution for the optimal n using the capacity expression (3.4) can not be derived which led us to obtain a closed-form expression using a numerical approach by means of MATLAB

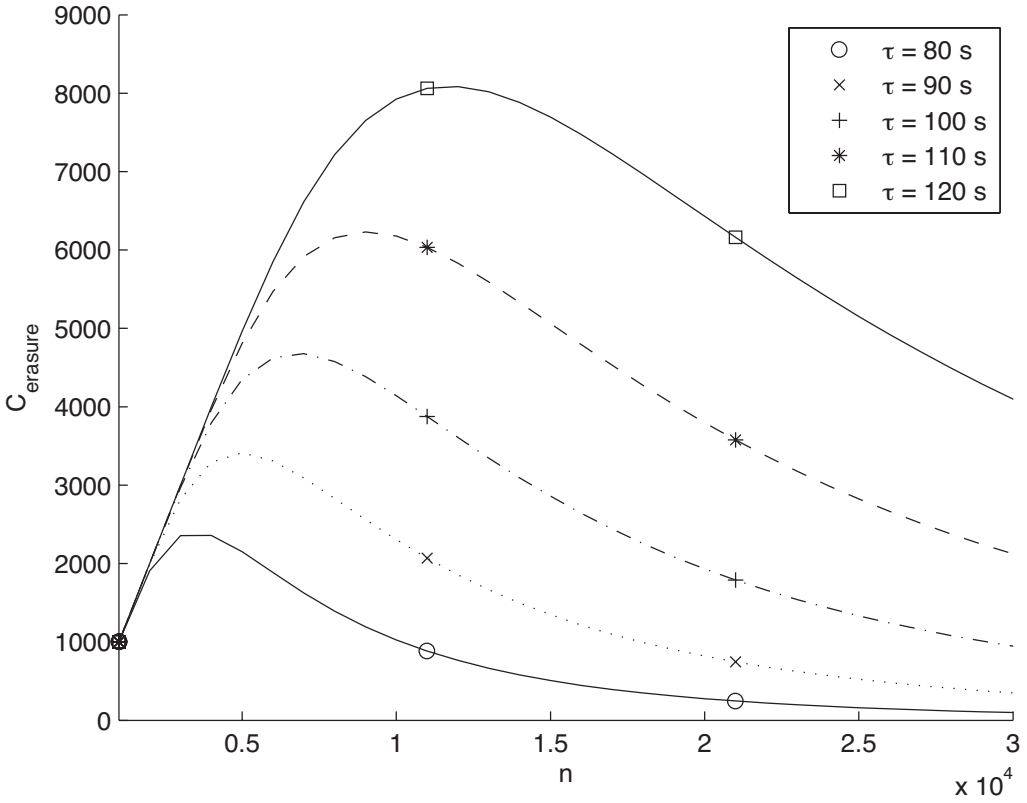

Figure 3.5: Capacity of molecular erasure channel for varying n (i.e., molecular size) with different lifetimes, τ

Optimization Toolbox and Surface Fitting Toolbox.

Firstly, optimal number of bits n is calculated and plotted in 3D with respect to the variation of two important parameters of optimization problem, namely, τ and N_M. Then, a surface is fitted on these data points as in Fig. 3.7. According to the results of surface fitting, a closed-form expression in the form of a polynomial of the third degree for each parameter is derived.

In Fig. 3.7, the optimal number of bits calculated numerically shown by the points and the surface fitted on them are illustrated. Using the parameters of the

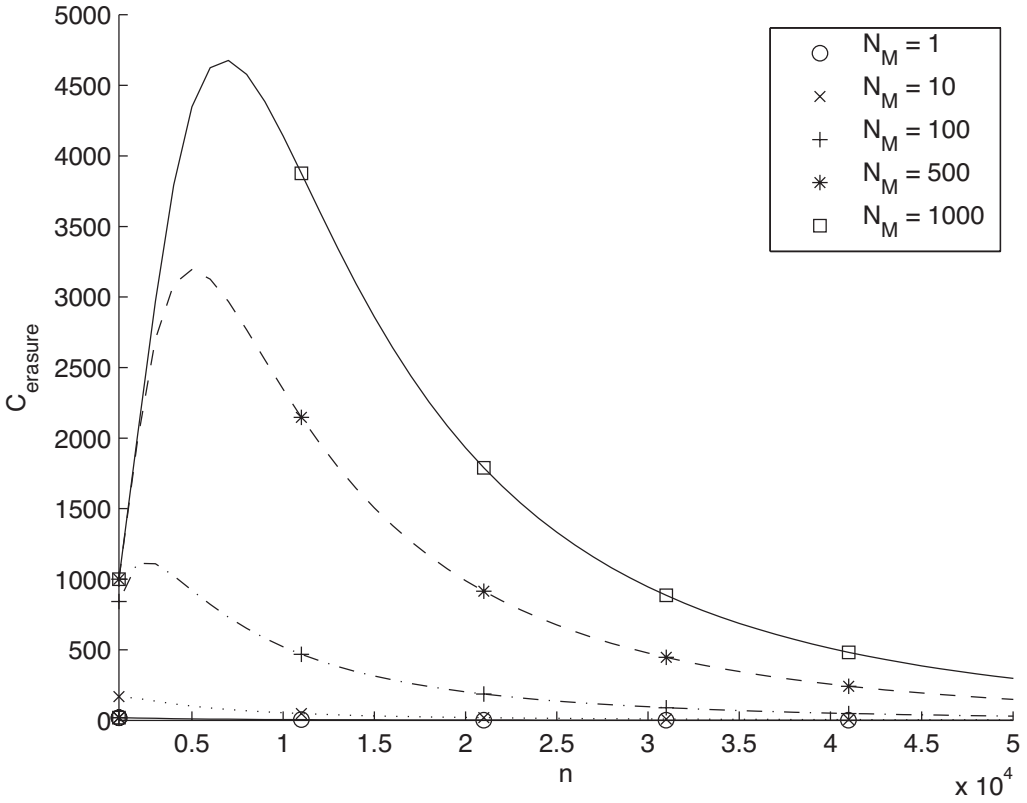

Figure 3.6: Capacity of molecular erasure channel for varying n (i.e., molecular size) with different number of redundant molecules, N_M

fitted surface an expression for optimal n is found as

$$\begin{aligned} n_{opt} &= 26.55 - 1.163N_M + 8.532\tau + 0.0023N_M^2 \\ &+ 0.012N_M\tau - 0.3019\tau^2 - 8.758 \times 10^{-7}N_M^3 \\ &+ 4.362 \times 10^{-5}N_M^2\tau - 0.00028N_M\tau^2 + 0.0024\tau^3 \end{aligned} \quad . \tag{3.6}$$

Besides finding the optimal number of bits encoded in a molecule in terms of the lifetime of the molecule τ and the number of redundant molecules N_M, we should also assess the feasibility of the described communication system. As the messenger molecules suggested in this study should operate in human blood, they should be able

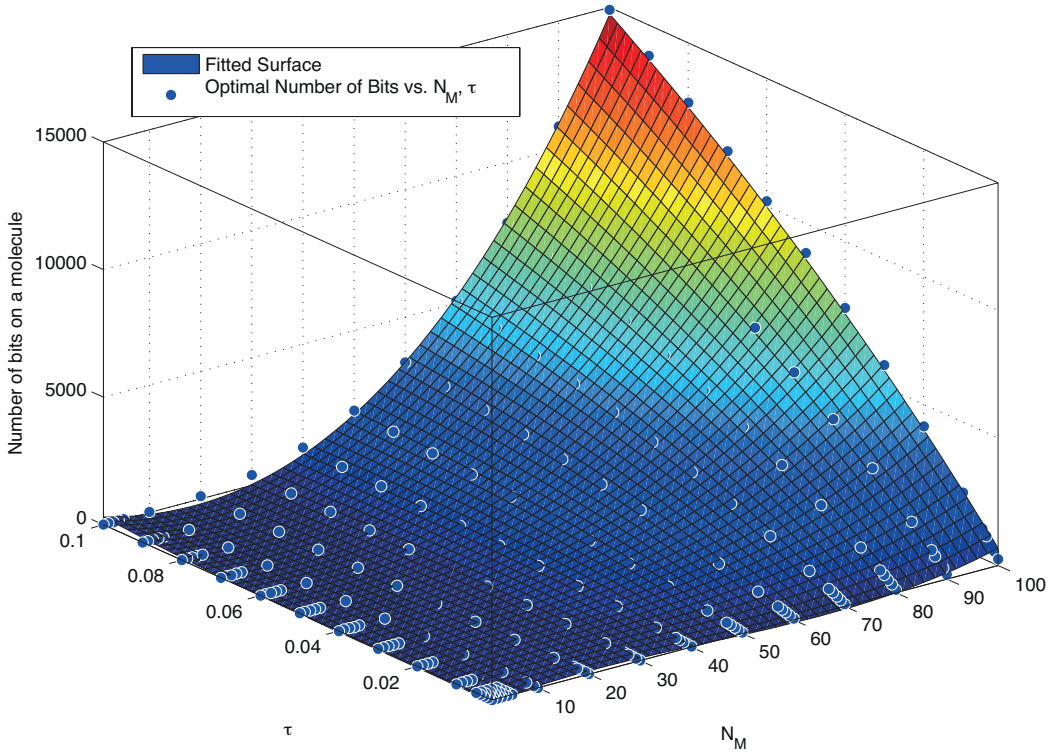

Figure 3.7: The fitted surface for the optimal number of bits, n

to tolerate the body temperature. For example, fluorocarbons with $n < 5$ have boiling points below 37° C. Thus, the messenger molecules should have at least $n = 5$ bits. During the phagoctosis of the messenger molecules by the immune system agents, molecules with n larger than 10^6 causes loss of phagocytic functions of these agents [5]. This phenomena settle upper and lower bounds for n. Considering Fig. 3.5 and 3.6, when the viscosity of the medium is set to the whole blood viscosity, the optimal number of bits lies between 0.25×10^4 and 1×10^4. These values satisfies the feasibility conditions stated previously.

Chapter 4

FORWARD ERROR CORRECTION FOR MOLECULAR NANONETWORKS

Molecular communications allows nanomachines to communicate with each other to form nanonetworks through sending and receiving molecules. The information is disseminated by varying the concentration or type of messenger molecules diffusing in the propagation medium. In this regard, we propose a messenger-based molecular communication model where information is encoded on the atoms of polyethylene molecules in the form of $CH_3(CHX)_mCH_2F$, where X is replaced either by an H or F atom, representing 0 and 1 bits, respectively. The propagation of the molecules is modelled as a Brownian Motion. Using Molecule Shift Keying modulation , our analysis focuses on analysing the bit error rate-power trade off of this channel and proposing simple forward error correction mechanisms trying to achieve the capacity via linear block codes.

4.1 Introduction

The scientists now are always trying to miniaturize electro-mechanical devices. However, at nanoscale the traditional methods are not working with the dynamics of particles at atomic level. Thus, new paradigms are needed to analyse and design at nanoscale. To this end, molecular communication is proposed as a novel communication at nanoscale enabling nanomachines to communicate with each other to form nanonetworks.

Molecular communication relies on the exchange of particular molecules between the transmitter nanomachines and receiver nanomachines which can be either naturally existent nanomachines such as biological cells or artificial nanomachines such as MEMS. By adjusting the concentration, the type or the arrival time of the molecules, the transmitter encode bits on the molecules that are released to the medium. Upon release, molecules propagate by diffusion following Brownian motion rules. When arrived to the receiver, the information embedded on the molecule is decoded.

Due to its size, nanomachines have very serious limitations on its functional capabilites and energy budget [1]. Therefore, it is crucial to use the resources efficiently for communication purposes. In this study, we propose a forward error correction mechanism for molecular communication to save from the transmission energy in expense of increased complexity for encoding and decoding.

Existing works on molecular communication concentrates especially on channel modelling for capacity and noise analysis for molecular communication by diffusion [9, 19, 55, 57]. However few of them deal with error compensation [58, 59, 60]. All three of these studies propose Forward Error Correction (FEC) as the error correction mechanism. FEC is more suitable for the molecular communication paradigm compared to other techniques such as Automatic Repeat Request (ARQ). Because of the stochastic nature of the diffusion process, message propagation delays are long and highly varying. If an ARQ method is used, the receiver should send acknowledgements to the transmitter through the same channel in reverse direction. Hence, acknowledgement messages are also subject to the long and varying propagation delays that doubles the delay and increases the probability of acknowledgement losses which is another error source absent in FEC.

In this study, the messenger-based molecular communication model described in Chapter 2 is considered. In this model, information is encoded on the atoms of polyethylene molecules which are in the form of $CH_3(CHX)_mCH_2F$, where X is re-

placed either by an H or F atom, representing a 0 and a 1 bit, respectively. The model is inspired from the pheromone release and detection processes by which animals like insects carry out chemical communication [56].

Similar to communications by pheromone release and reception, encoded polyethylene molecules are assumed to be released into the medium by sender nanomachines and left to propagate following a Brownian Motion process to the receiver nanomachine. Brownian Motion of molecules has a very stochastic nature. This communication model suffers from long propagation delays because of molecules moving in all directions in the propagation medium which causes a low probability of reception at the receiver. Furthermore, during this long propagation time, the probability that messenger molecules interact with other chemical compounds present in the propagation medium increases. Consequently, the messenger molecules may change their chemical structure, so the message carried on them may be totally or partially destroyed. For example, one H atom of m coded atoms of $CH_3(CHX)_mCH_2F$ may be switched to F or vice versa.

To overcome these bit errors, we propose a forward error correction scheme which uses (n,k) linear block codes of which adds redundant bits to the message encoded on a molecule to increase the achievable rate of the system. The blocks of length k are mapped to blocks of length n. However, it is not a trivial problem since including forward error correction does not always improve the bit error rate. For forward error correction either larger molecules or new molecules are needed to carry the redundant bits which in turn increases the uncertainty in molecule motion and delay. Thus, it is worth to analyse the effect of forward error correction in molecular communication systems and observe the tradeoff between the bit error rate and power.

The remainder of this chapter is organized as follows. In Section 4.2, the molecular communication model with multiple bit carrying molecules is introduced. The channel model and the capacity calculation are given in Section 4.3. The forward

error correction scheme is proposed in Section 4.4.

4.2 Molecular Communication Model

The molecular communication model adopted in this study is based on the model described in 2. The point-to-point communication between the transmitter and receiver nanomachines can be divided into 5 main processes, namely; information encoding process, transmission process, propagation process, reception process and information decoding process.

4.2.1 Information Encoding Process

The transmitter nanomachine generates fluorinated polyethylene molecules in the form $CH_3(CHX)_mCH_2F$ as messenger molecules carrying m bits of information. Here, X stands for either an H or F atoms, representing the 0 or 1 bits, respectively. The information encoding order is provided by the distinctive head and tail of the molecule, i.e., CH_3 and CH_2F.

For the structure of the molecules we can further assign some rules. A polyetylene molecule can carry the encoded atoms only in one side of the molecule and the other side is padded with H atoms so that the receiver nanomachine knows which side is coded and avoid the confusion which may arise from the longitudinal symmetry of the molecule. Considering this, the information density of the polyethylene molecule becomes $d_{message} \sim 26\ bits/nm^3$ which is significantly higher than the similar molecules used for information storing. For example, a more common molecule, DNA, has an information density of $\sim 1\ bit/nm^3$ [5].

The information carrying capacity of a single molecule increases with increasing m, in exchange for a larger molecule size which slows down the diffusion of the molecule. Hydrofluorocarbon molecules with m >20, as in the polyethylene molecule in con-

sideration in this study, can be folded into a maximally compact spherical shape in order to ensure a high packing density [50] during preparation for transmission. The diffusion coefficient for spherical particles through liquid is expressed by the Einstein-Stokes equation [53] as

$$D = \frac{k_B T}{6\pi\eta r}, \tag{4.1}$$

where k_B is the Boltzmann's constant, T is the absolute temperature and η is viscosity and r is the radius of the nanomachine.

Molecule Shift Keying (MoSK), a molecular modulation technique introduced in [23], can be exploited for the information encoding process of this study. This modulation scheme requires 2^m different molecules to represent m bits of logical 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. This process is similar to orthogonal signalling used as a modulation technique by conventional electromagnetic communication. Each different molecule corresponds to one of the $2^m = M$ symbols. An example $m = 2$ bit constellation diagram for binary MoSK is shown in Fig. 4.1 to visualise the fluorinated polyethylene molecule [23]. In our case, m can reach up to the order of 10^4, corresponding constellation diagrams are similar to the diagram in Fig. 4.1.

4.2.2 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 the nanomachine. This emission process is uniformly distributed over the aforementioned spherical boundary, called the emission boundary. If a living cell is chosen as the nanomachine, emission boundary is the cell membrane.

Since the messenger molecules are assumed to propagate by Brownian Motion, the

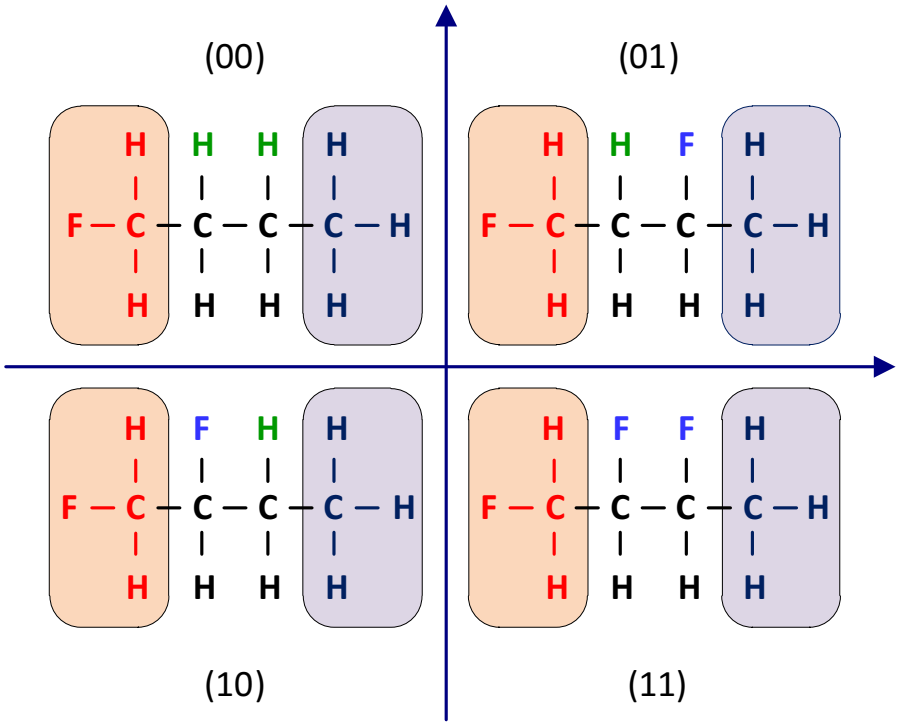

Figure 4.1: Diagram for binary MoSK modulation, $m = 2$.

probability that a single messenger reaches the receiver in a given time is very small. Hence, for the purpose of reliability, the transmitter emits redundant copies of the molecule, namely N_M such copies, for each message in order to raise the reception probability. The transmitter nanomachine does not prepare the molecules in advance, and does not store the molecules generated for future use.

Emission of the molecules takes place instantaneously, i.e., the concentration of the messenger molecule in the medium is increased abruptly in a short amount of time. This model is inspired from the instantaneous emission of pheromones in animals in alarming situations such as threats from predators and enemies, injured conspecifics, exposure to toxic compounds occurs [31].

4.2.3 Propagation Process

Messenger molecules released from the transmitter propagate in the fluid medium by diffusion. The random motion of the messenger molecules is modelled as Brownian. We assume that the total concentration of emitted molecules are much lower than the concentration of all fluid molecules. Therefore, the interactions between molecules are neglected and the movement of each molecule is assumed independent. Considering these assumptions, we can express the concentration of the molecules by Fick's law of diffusion [54].

For instantaneous emission of the messenger molecules described in Section 4.2.2, the concentration of the messenger molecules in space with respect to time can be found by

$$U(r,t) = \frac{N_M}{(4\pi Dt)^{\frac{3}{2}}} \exp\left(\frac{-r^2}{4Dt}\right), \tag{4.2}$$

where D is the diffusion coefficient and r is the radius of the spherical messenger molecule [49].

The first hitting time of an emitted molecule to a spherical surface at a distance d away from the emission boundary, denoted by t, is distributed according to an inverse Gaussian probability density function [55], i.e.,

$$f(t) = \frac{d}{\sqrt{4\pi Dt^3}} \exp\left(\frac{-d^2}{4Dt}\right), \;\; t \geq 0. \tag{4.3}$$

The random variable t can also be defined as the propagation delay of a single molecule for a distance d.

4.2.4 Reception Process

Receiver nanomachine has specific receptors which bind to the messenger molecules arriving to their vicinity. When a messenger molecule hits the boundary of the receiver, it is assumed to be instantly captured for decoding. Furthermore, the captured molecules are not re-emitted to the medium.

Since the messenger molecules randomly propagate in the medium in all directions, all the molecules emitted from the transmitter do not reach the receiver. Besides, the messenger molecules can be degraded by the propagation environment. Only a part of them arrive to the boundary of the receiver. Thus, the transmitter releases N_M copies of the messenger molecule, to increase reliability by redundancy. The booster effect on channel capacity of using extra molecules in a molecular channel where the information is encoded in the concentration of the molecules is illustrated in [55]. We assume that reception of only one of the N_M molecules released for a single message is sufficient for decoding the message.

4.2.5 Decoding Process

The decoding process takes place after the reception of the incoming messenger molecules. By exploiting the special structure of the molecule described in Section 4.2.2, the receiver reads the information encoded on the incoming molecules. The head and tail structure enables the receiver to know from which end of the molecule it should start decoding. Furthermore, since only one side of the molecule is encoded as described in Section 4.2.2, the receiver also knows which side should be decoded.

The molecule captured by the receiver is decoded by the demodulation of the incoming molecule generated according to MoSK presented in Section 4.2.2. The antennas in the olfactory systems of the moths [34], which can identify thousands of different pheromone molecules, may be used as the decoder. Another alternative decoding scheme is reading the molecule bit by bit. The difference in interaction energies between the coded H and F atoms and the boron atom, B, of a C_5H_5B or $C_3H_3N_2B$ probe reveals the type of the coded atom [35].

4.3 Channel Model

Using the communication model proposed in Section 4.2, we consider a data transfer among a transmitter and a receiver nanomachine which are separated by a distance d and put forward a channel model for the messenger based molecular communication based on the channel model described in Section 3.3. But here, we consider that time is slotted to be able to compare our results with [59] which studies also FEC for molecular communication but for modulation by concentration. Thus, the channel is assumed to be an M-ary symmetric channel without any erasures. The time slot is adjusted such that the probability of successful reception goes to 1.

As described in Section3.3, the message-carrying fluorinated polyethylene molecules are generally biocompatible, even though a thorough study for toxicity levels of different types of polyethylene molecules is still required [5]. Some of the fluorinated polyethylene molecules such as Fluosol-DA are FDA approved to be used in artificial blood formulations [51]. Thus we consider that the proposed communication model operates in human body transferring information by fluorinated polyethylene molecules propagating in blood without harming the human body.

We stated in Section 4.2 that the modulation by molecule diversity first introduced in [23], i.e., Molecule Shift Keying (MoSK) is used in this study. We assume that the modulation is done using m atoms encoded in one molecule representing 1 bit of information which corresponds to using $M = 2^m$ different molecules which corresponds to M different orthogonal symbols.

Although the polyethylene molecules are considered stable and chemically inert [51], there are two error sources causing a symbol error. Symbol error occurs when at least one of the atoms carried on the messenger molecules is altered by the effects of the propagation environment when the substances in blood react with the messenger molecule and degrade the molecule structure by changing its atoms. Although

polyethylene is considered stable, there is a certain probability β that one of the bits is flipped, i.e., H and F atoms are interchanged. The second error source is intersymbol interference ISI caused by the remaining molecules from the transmission taken place in the previous time slot. Theoretically, all the transmissions done in all the previous time slots contribute to the ISI. However, for molecular communication by diffusion framework it has been shown that a very large portion of ISI is caused only by one previous time slot. Hence, we only consider the residual molecules released in the previous slot but arriving in the current time slot.

To find the relation between the bit error rate and the transmission power we first calculate the symbol errors caused by the environmental effects denoted with Q_E. To do so, first p, the probability that a molecule reaches the receiver before the end of the time slot, i.e., before τ, should be found by

$$p = \int_0^\tau f(t)dt \tag{4.4}$$

where $f(t)$ is the probability density function of first hitting time of the molecule to the receiver, given in (4.3). Then, the successful delivery of one of the N_M released molecules before τ is calculated by

$$p_{symbol} = 1 - (1-p)^{N_M}. \tag{4.5}$$

Then, the probability of successful delivery considering the environmental effects is calculated as

$$Q_E = p_{symbol} * (1-\beta)^m. \tag{4.6}$$

For the second error source, ISI, we consider the residual molecules from the previous slot as they are the only ones effecting the current symbol. The probability that a molecule released in the previous slot arrives in the current time slot can be found by

$$q = \int_\tau^{2\tau} f(t)dt. \tag{4.7}$$

Hence, the probability of error brought by ISI becomes

$$P_{ISI} = (1 - (1 - q)^{N_M})(1 - p)^{N_M}. \tag{4.8}$$

Then, the probability of total symbol error P_E is expressed by

$$P_E = 1 - Q_E + P_{ISI}. \tag{4.9}$$

Since we use an M-ary modulation we use the following relation to find the bit error rate using probability of symbol error

$$P_b = \frac{2^{m-1}}{2^m - 1} P_E, \tag{4.10}$$

which is valid for modulation by orthogonal signalling as in our case [62].

After expressing the bit error rate, we find the power required for transmission. In [63], it is shown that the transmission power is directly proportional to the number of bits released for that message. Thus, hereafter we use the number of molecules N_M as the measure of power.

In Fig. 4.2, the BER-power tradeoff is shown for 3 typical distances, namely, for $d = 30, 40, 50\ \mu m$. For the same power level, the bit error rate increases as the distance between the transmitter and the receiver increases. The shape of the figure is similar to the bit error plane of [59] shown in Fig. 4.3 which studies molecular communication with concentration modulation.

4.4 Forward Error Correction by Linear Block Codes

Forward error correction is used to increase the transmission reliability and decrease the transmission power in expense of power and complexity for coding and decoding the messages. When the power consumption for error control coding exceeds the saving in the transmission power, error control coding becomes dysfunctional.

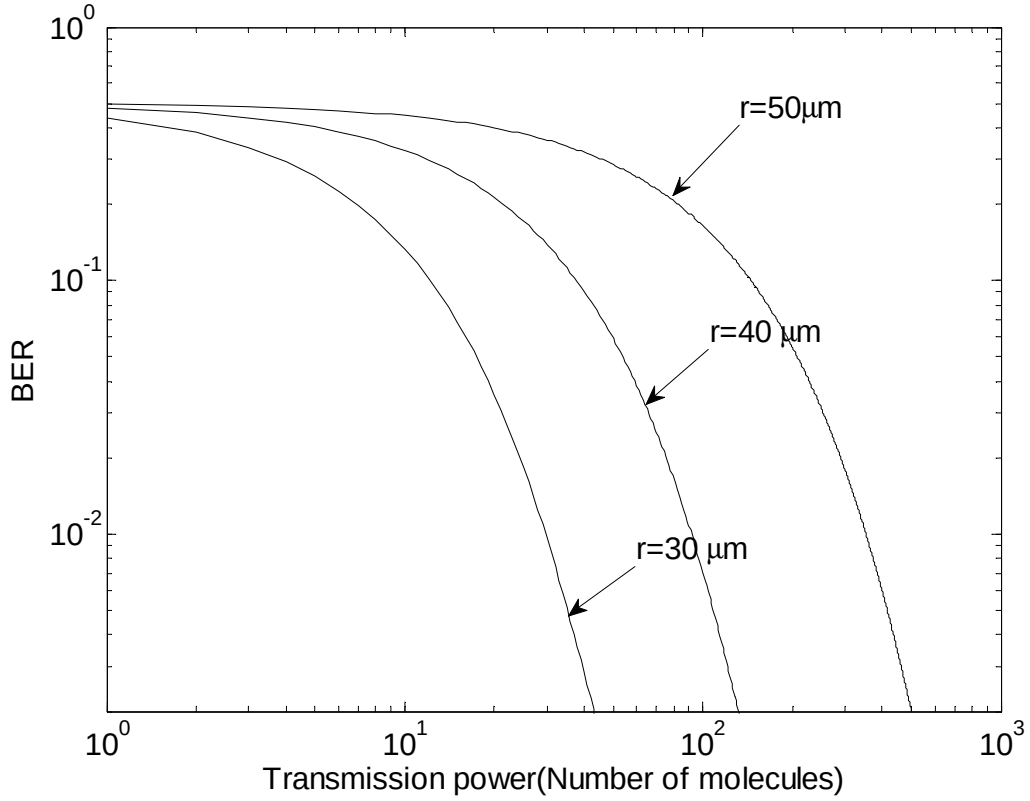

Figure 4.2: BER vs N_M for distances $d = 30, 40, 50$ μm.

Since complex computations for coding and decoding are beyond the capabilities of nanomachines, simple coding techniques requiring less energy are preferred.

In addition to the power aspect, the effectiveness of coding should also be assessed in the sense of transmission reliability. When the length of the codewords increases with coding, the molecule carrying the message gets larger hence diffuses slower. After a certain molecule size, i.e, codeword length, the errors caused by the slow diffusion overweighs the gain of error correction. Thus, it is valuable to find out in which cases error control coding is advantageous and in which cases coding does not bring any gain.

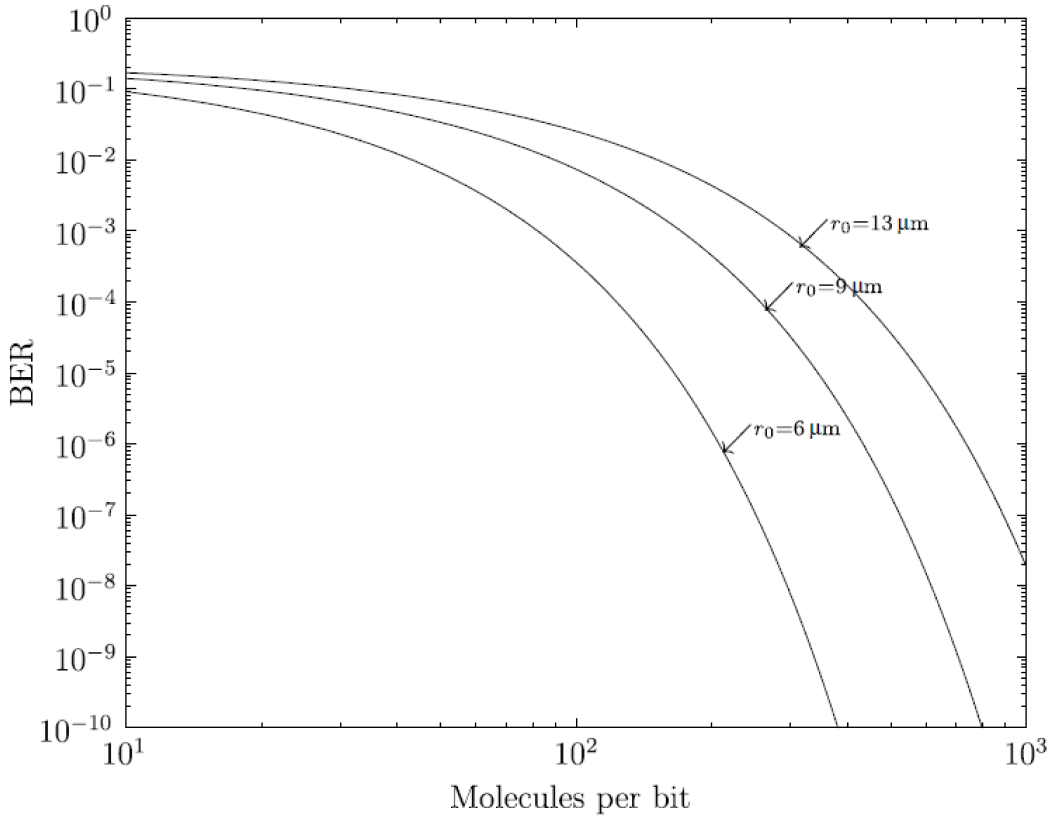

Figure 4.3: BER vs Number of Molecules for modulation by concentration [59].

In this study, we consider using simple linear (n,k) block codes where $n = 2^a - 1$, $k = 2^a - a - 1$ and a takes values $3, 4, 5$. When the error correction codes are used, the transmission power is scaled by the coding ratio n/k. To compare the performances of uncoded and coded transmissions, we need to find the bit error rate expression for the coded case. For linear block codes an approximate expression is given as

$$P_b^{coded} = \frac{1}{n} \sum_{j=t+1}^{n} j \binom{n}{j} {P_b}^j (1 - P_b)^{n-j}, \tag{4.11}$$

where t is the maximum number of bit errors that can be corrected using the code

and P_b is the bit error rate of the uncoded case.

The resultant bit error rates are illustrated in Fig. 4.4 for different transmission power levels represented by the number of molecules sent for one transmission. Fig. 4.4 show that coding is not efficient if the transmission power level is low. However, coding significantly improves the bit error for larger transmission powers. Raising a, i.e., using longer codes and at the expense of increased coding and decoding complexity, we can achieve lower BER for the same power level which corresponds to using the same number of molecules for one transmission. In Fig. 4.5, similar results are obtained for modulation by concentration.

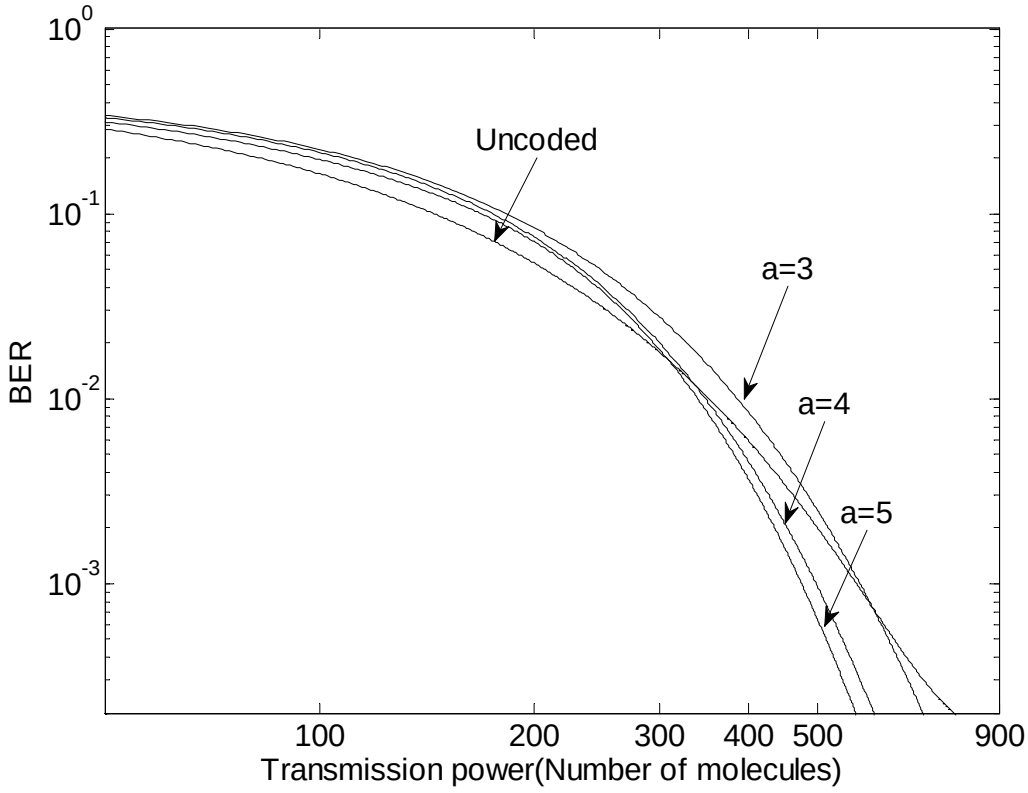

Figure 4.4: BER vs Number of Molecules for $a = 3, 4, 5$.

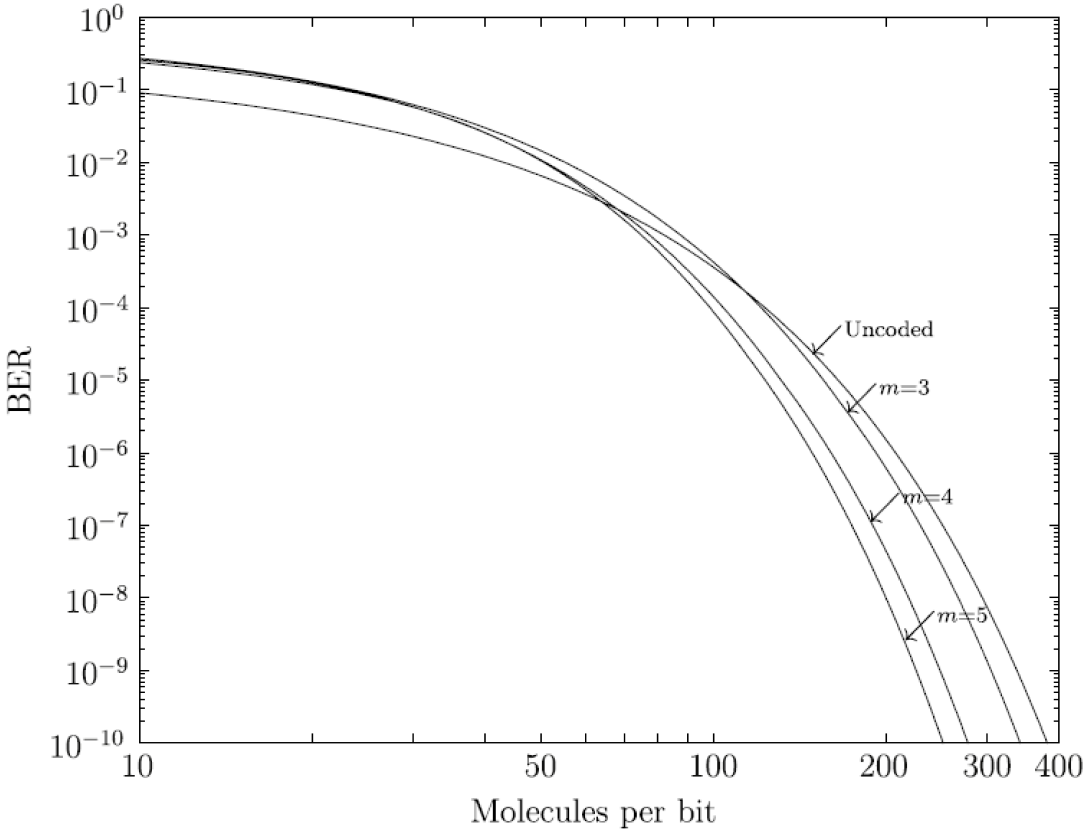

Figure 4.5: BER vs Number of Molecules for modulation by concentration [59].

Despite the limited computation capacity of nanomachines, simple channel coding operations for forward error correction may be feasible through molecular gates [43]. In this study we consider the simplest traditional channel coding algorithms that we assume within the potency of nanomachines. However for the utmost performance for error control coding in molecular communication, algorithms especially designed for molecular communication taking into account the characteristics of nanonetworks should be designed.

Chapter 5

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

The development of nanotechnologies will continue to grow and give the superiority to the ones using and controlling it in almost every domain from economics, homeland security, environmental protection and sustainability to biomedicine. To engage nanotechnologies in these real life application areas, nanocommunication techniques are crucial since the basic functional units, nanomachines which are operating in a few hundred nanometers environments need to communicate with each other to form nanonetworks performing complex macroscale tasks.

Molecular communication is a promising technique to establish communication at nanoscale in which molecules are used to carry messages between nanomachines. In this thesis, we introduce a new communication model for molecular communication which exploits molecule diversity. An information theoretical analysis of this channel is conducted to investigate the rate-delay trade-off, the capacity and the bit error rate. Our aim in this thesis is to find the feasible conditions and techniques to realize a molecular communication system. Furthermore, we derived analogies between the conventional electromagnetic communications and the emerging molecular communication fields to exploit the techniques used in conventional networks such as network coding and forward error correction for optimizing the performance of molecular networks.

In the following sections, we summarize our contributions and state research chal-

lenges and open issues for molecular communication in nanonetworks.

5.1 Contributions

In this section, we give a brief summary of the contributions of each chapter.

5.1.1 Rate-Delay Tradeoff with Network Coding in Molecular Nanonetworks

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 work constitutes a basis for rate and delay optimization of future nanomolecular frameworks.

5.1.2 Molecular Channel Model with Multiple Bit Carrying Molecules

In this study, a molecular communication scheme with multiple bit carrying fluorinated polyethylene messenger molecules is presented. The communication channel with Brownian propagation is modelled as a block erasure channel and its capacity

expression is derived. Numerical results reveal that when parameters such as the number of redundant molecules and the slot length are properly tuned, very high capacities are achievable. Optimal number of bits in capacity sense is approximated as a function of these parameters. Achievable capacity and the polyethylene biocompatibility makes the proposed model a candidate for molecular communication systems for nature and human body.

5.1.3 Forward Error Correction for Molecular Nanonetworks

In this study a molecular communication scheme where the messenger molecules carry multiple bits on fluorinated polyethylene molecules is presented. The communication channel where messenger molecules obey Brownian Motion is modelled as a q-ary symmetric erasure channel and the capacity expression is derived. Then, several forward error correction mechanisms are proposed such as Hamming and Golay codes to improve this capacity. These kind of studies pave the way for establishing analogies between conventional electro-magnetic communication and molecular communication.

5.2 Future Research Directions

Molecular communication is a new communication paradigm which needs elaborate investigation. Despite the numerous theoretical studies, only a few experimental studies are conducted. Thus, the feasibility is the major concern for future research. Especially, an interdisciplinary approach combining ICT with biology, chemistry and material science is vital. Inspired by inter-cell and intra-cell molecular communication systems of biological entities, molecular communication by diffusion, bacteria nanonetworks, artificial neural networks are some of the proposed solutions under investigation.

In particular, for molecular communication by diffusion which was the main sub-

ject of this thesis, research challenges include the development of transmitter and receiver nanomachines, testbeds and simulation tools, the knowledge transfer from conventional communication systems to build communication architectures and protocols for molecular communication, design&analysis of communication channels capable of operating under the limited resource constraints.

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