B. TECH. PROJECT REPORT

On

Performance Analysis and Optimization of Relay-Assisted Molecular Communication with Line Transmitter

BY

GUNJAN PATIL

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Performance Analysis and Optimization of Relay-Assisted Molecular Communication with Line Transmitter

A PROJECT REPORT

Submitted in partial fulfillment of the
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of
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Submitted by:
Gunjan Patil

Guided by:
Dr. Prabhat Kumar Upadhyay
Assistant Professor
Discipline of Electrical Engineering

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CANDIDATE'S DECLARATION

I hereby declare that the project entitled **"Performance Analysis and Optimization of Relay-Assisted Molecular Communication with Line Transmitter"** submitted in partial fulfillment for the award of the degree of Bachelor of Technology in **Electrical Engineering** completed under the supervision of **Dr. Prabhat Kumar Upadhyay, Assistant Professor, Electrical Engineering, IIT Indore** is an authentic work.

Further, I declare that I have not submitted this work for the award of any other degree elsewhere.

Gunjan Patil
B.Tech. IV year
130002013
Discipline of Electrical Engineering
Indian Institute of Technology Indore.

CERTIFICATE by BTP Guide

It is certified that the above statement made by the students is correct to the best of my/our knowledge.

Dr. Prabhat Kumar Upadhyay
Assistant Professor
Discipline of Electrical Engineering
Indian Institute of Technology Indore.

Preface

This report on "**Performance Analysis and Optimization of Relay-Assisted Molecular Communication with Line Transmitter**" is prepared under the guidance of *Dr. Prabhat Kumar Upadhyay*, Assistant Professor, Electrical Engineering, IIT Indore.

Through this report, an accurate and reliable wireless communication system at nanoscale is illustrated by introducing the field of molecular communication via diffusion, explaining the relay-assisted molecular communication model in detail with the help of a pictorial 2D model, the unique features of the model, the theory on which this type of communication is based, the error that impairs the performance of the system and the ways by which this error can be minimized. Lastly through numerical results, the impact of the unique features of the model on the error probability and thus, on the system performance is shown. In this report, meaningful insights are obtained through numerical results which are different from the research work produced till now.

The content is explained in a lucid manner with the best of my abilities and knowledge. Furthermore, 3-D models, figures and tabulated data is added to make the content of this report more illustrative.

Gunjan Patil
B.Tech. IV Year
Discipline of Electrical Engineering
IIT Indore

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Finally, I offer sincere thanks to everyone else including my family members, friends and colleagues who knowingly or unknowingly helped me complete this project.

Gunjan Patil
B.Tech. IV Year
Discipline of Electrical Engineering
IIT Indore

Abstract

There has been much advancement in the field of nanotechnology, bioengineering and synthetic biology over the past decade, yet the problem of engineering a reliable communication system between tiny devices is still an open problem. At the same time, despite the prevalence of radio communication, there are still areas where traditional electromagnetic waves find it difficult or expensive to reach. Points of interest in industry, cities, and medical applications often lie in embedded and entrenched areas, accessible only by ventricles at scales too small for conventional radio waves and microwaves, or they are located in such a way that directional high frequency systems are ineffective. Inspired by nature, one solution to these problems is molecular communication (MC), where chemical signals are used to transfer information. Although biologists have studied MC for decades, it has only been researched for roughly ten years or more from a communication engineering view. Significant number of papers have been published to date, but owing to the need for interdisciplinary work, much of the results are preliminary.

In this project, a reliable molecular communication system is achieved by deriving the error that occurs in such a model and then improving the performance of the system by proposing an optimization problem with respect to some parameters which decide the rate of error incurring in the system. Different models can be proposed in this type of communication system .But based on which model can be better realized in nature is the one proposed in the report. Thus, in this report, a relay-assisted and a flow-assisted diffusion-based molecular communication system inside a 1D medium exposed to all types of noises is considered in which the molecules will have a definite life expectancy and the components – transmitter, relay and receiver have finite linear volume. After such a model is considered, the end-to end error probability of the source-relay-destination system as a function of the detection threshold at destination is derived. Further, an optimization problem formulated with respect to this threshold variable is solved using available methods in MATLAB and finally, the performance of the system is evaluated on various parameters that come into picture due to various features proposed in the relay-assisted molecular communication model. The report finally concludes with the analysis of overall reliability of the proposed model and the future scope of the project.

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Chapter 1

Introduction

This chapter highlights the background required to understand this molecular communication domain related project and the motivation behind doing this project and the objectives of the project.

1.1 Background

Since the inception of machines on nanoscale, the requirement for transfer of data at such scale has emerged. This is where nano communication steps in. It, inspired from biological paradigms, uses molecules to transfer data/information. Biocompatibily as well as efficient use of energy are the prime benefits of molecular communication (MC) over traditional methods. This can allow nanomachines to achieve macro-scale results by efficient communication between the machines. It has many novel applications especially in biomedical field, along with environmental and industrial applications. These potential applications and the need for growing field of nano communication have been the motivational aspects of this project. The motivation behind this project is to make significant contribution in the advancing field of molecular communication. To understand further what motivated to implement the proposed MC model, it is necessary to get an overview of MC and understand different components essential to carry out this communication.

1.2 Overview of Molecular Communication (MC)

In general, any communication system consists of three components: transmitter, channel and receiver. The transmitter generates a signal containing the information that needs to be transmitted which propagates through the channel and reaches the receiver where the messages is extracted from the signal. Thus a message is transmitted from one place to another in a communication system.

Figure 1.1 shows some of the physical components that are required to implement an MC system.

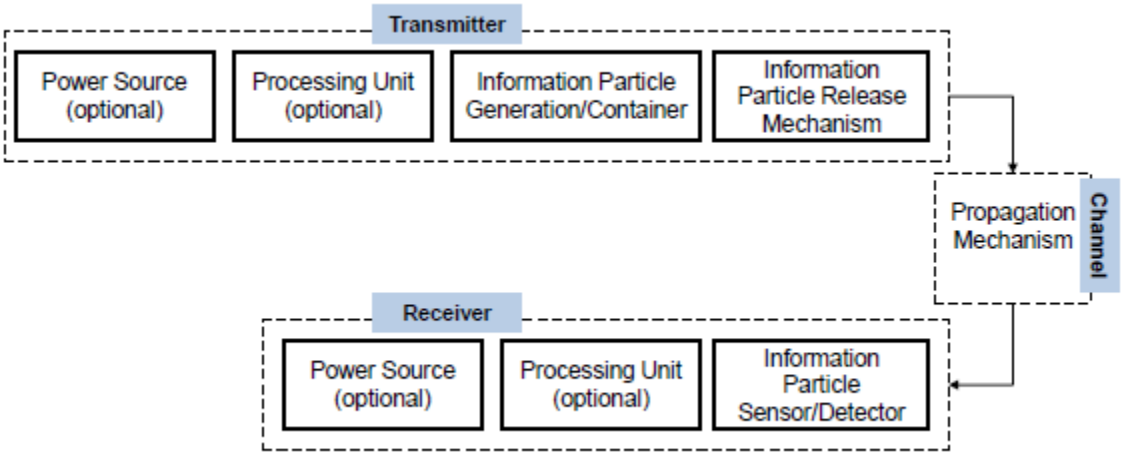


Fig. 1.1: *The physical components of a molecular communication system.*

A transmitter needs many physical processes to generate the required signal and also to store the particles needed for transmitting information. A processing unit is required to control how the different components of the transmitter work together. It runs on some sort of power supply, either chemical or electrical, and help manage the working of transmitter like controlling the release of particles. At the transmitter, a physical process is required for generation or storage of information particles. Biological transmitters can get energy from their environment and synthetic electrical chips as microcontrollers need electrical power supply.

It has been established, in literature, that information can be modulated using different properties of molecules. Based on the parameters used to modulate the information, like concentration or identity of molecules or the frequency of signal, modulation techniques can be divided into following three main kinds:

1. Concentration Shift Keying (CSK) – If number of molecules released is used to encode the information then it is called concentration shift keying. In traditional systems, this method is called on-off keying. Different number of molecules represent different bits. As an example, 1000 molecules can be sent to send the bit 1 while zero molecules can be sent to denote the bit 0.

2. Molecular type Shift Keying (MoSK) – If the types of particles is used to encode the information it is called molecular type shift keying. In this type of encoding, different types of molecules are used to transmit different symbols. As an example, molecules of type A can be transmitted to symbolize the bit 1 and molecules of a different type B can be transmitted to symbolize the bit 0.
3. Release Time Shift Keying – If the time of release of molecules, within a symbols duration, is used to encode the information then it is called release time shift keying. In this method, an example of such encoding is Pulse Position Modulation (PPM). In PPM, a large number of molecules are released either in the first half or the second half of the symbol duration to signify two different symbols. As an example, releasing molecules in first half may signify the bit 1 being transmitted and that in the second half may be considered as the bit 0.

When the particles enter the channel, they are transported to the receiver using one of the several mechanisms. They can either be transported using a diffusion channel or a flow based channel. A transport system with motors made of molecules can also be engineered to ensure the transportation of information from the transmitter to the receiver. When the molecules arrive at the receiver, some sort of a detector is needed to sense a measurable property of the particles in order to receive the signal. Either concentration, time of arrival or any other feature of the particles can be used depending upon the transmitting system used. A processing unit may also be needed for decoding the information from the signal received. Also, a power source of some kind can be needed for the operation of receiver.

Unlike the traditional communication systems - where open space or a wire is used as the channel with either electric currents or electromagnetic waves being used as the transmitted signal – in MC, molecules are used as the chemical signals to carry information. The size of these particles varies in a few nanometers to micrometers range. Either biological compounds or synthetic compounds are generally used as the information particles. For instance, proteins or gold nanoparticles can be used as information particles. The channel in such communication, being aqueous or gaseous environment, is such that it allows these small particles to propagate freely.

Typically, in communication systems, noise creeps into the transmitted signal and distorts it. In radio based system this is mainly due to fading or interference of the transmitted electromagnetic waves. In MC, the sources of noise can be as follows:

- random propagation (diffusion) noise
- transmitter emission noise
- receiver counting/reception noise
- environment noise such as degradation and/or reaction
- multiple transmitters

After the receiver receives the signals, it demodulates the information and detects the symbols. These symbols are then passed on to channel decoder, which decodes these channel symbols and preferably also removes some of the errors introduced during transmission. Its output is then passed on to a source decoder which decodes the information depending on what encoding has been used at the source, it then estimates the information that has been transmitted from the transmitter. The estimation of symbols can be inaccurate and this is called symbol error probability. If bits are used as symbols then this probability is called bit error probability. The correct estimation determines the performance of the system and hence its success or failure.

In nature, MC is present at every scale from distances in order of nanometers to the order of meters. In microscale MC, neurotransmitters inside cells are example of short range communication while motor proteins which carry cargoes are example of mid-range communication. In macroscale MC, hormones in blood vessels are transmitted over meters of distance. The physical properties of matter change from macroscales to microscales. In this report, the referred values for distance and other parameters are taken from the literature [2]. The range of the distance between nanomachines is in μm, hence microscale MC is considered and discussed in the next sub-sections.

1.2.1. Microscale Molecular Communication

One prominent mode of communication at small scales is utilizing the existing MC systems in nature. This communication is useful to achieve a communication network between nano devices at nano scale. The main components used in this communication are described below:

1. **Information particles**: Since the propagation depends on diffusion of information particles and the diffusion coefficient is dependent on the size and type of the particles, hence the structure and size of these particles affects the communication. Moreover, for reliable communication, these particles need to be chemically stable and robust against noise from other particles. Enzymatic attacks or varying pH affects can degrade the information particles. In biological processes, there are a lot of different types of information particles - including but not limited to - hormones, pheromones, neurotransmitters, intracellular messengers, and deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) molecules. Information particles can also be synthesized for specific purposes as demonstrated in drug delivery.
2. **Channel and Propagation**: For microscale MC, many different propagation schemes are possible for transporting information particles. These schemes include molecular communication via diffusion (MCvD) (such as calcium and pheromone signaling), diffusion with first hitting, flow assisted propagation, motor proteins motility over microtubules, microtubule motility over stationary motor proteins, and bacterial assisted propagation. The propagation scheme used in this model includes the first three propagation scheme because MCvD has shown to be both an effective and energy-efficient strategy in the literature [3]. The MCvD propagation method is illustrated in Figure 1.2.

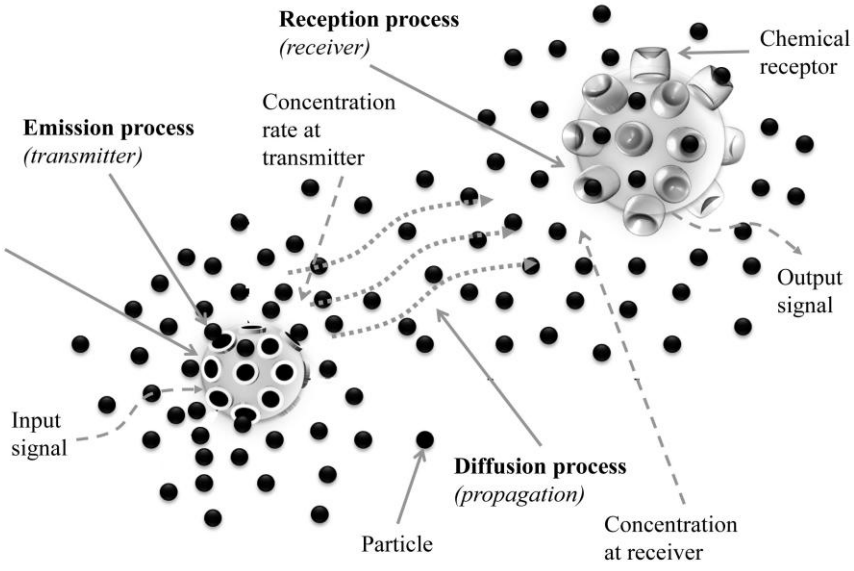


Fig. 1.2: Molecular Communication via Diffusion.

Generally, since the environment doesn't have flow currents, diffusion is the only method considered that helps in propagation of molecules. Although it has many advantages, being able to transport molecules without needing any external energy, it can be very slow as molecules propagate in Brownian motion. Hence flow assisted propagation is needed. The flow, if it is in the direction of transmitter to receiver then it is called a positive drift. Positive drift is most effective flow. It helps by speeding up the process of propagation. In nature, mainly, the information is received by removing it from the information molecules by either absorbing, binding or chemical reactions with the information molecules. Therefore, in most cases almost all the molecules contribute to the signal at most once. In other cases, it can still be ensured that each molecule contributes to the information only once by other mechanism like breaking down the received molecules into constituents. This type of process is modelled as first hitting process. In this type of modelling, the receptors remove the information particles upon detection as detection involves removal of the molecules from the environment. Hence this type of modelling is very handy.

Thus, the propagation scheme used in the proposed model is a combination of diffusion with first hitting via flow assisted propagation. The idea of flow assisted transmission can be supported by numerous healthcare applications of MC system such as the detection and monitoring cholesterol or disease precursors in the blood vessels.

3. **Transmitter/ Receiver Mechanisms and Components:** The transmitter and the receiver of microscale MC can be any machine in the microscale to nanoscale dimensions. For example, the transmitter and the receiver can be generated by modifying cells genetically [4], or by creating artificial cells [5]. In every method, the transmitter still needs to have at least the three components mentioned in the previous section: a unit for generation or storing information particles, a unit for controlling the release of information particles, and a central processing unit. Similarly, the receiver needs at least two components: a detection unit for sensing the information particles, and a processing unit for decoding and deciphering the intended message from the detection unit's measurements. Physically, the central processing unit of the transmitter and the receiver may be implemented by synthesizing logic gates and memory into cells as shown in [6]. The information particles can be generated by modifying a metabolic pathway of a biological cell, which then synthesizes and releases specific signaling molecules [7].

To control the release timing, a synthetic oscillator can be introduced into a cell [8], which with the help of the central processing unit acts as the release control module. Therefore, it is possible to have all the components of a transmitter synthesized into cells. Similarly, it is possible to synthesize receptors for a specific type of molecules into cells [9]. Therefore, it is possible to have all the components required for the receiver inside a synthetic cell. More sophisticated processing units can also be designed as shown in [10], using novel materials and spin waves (spin waves are propagating disturbances in the ordering of magnetic materials). Finally, it is possible to develop the transmitter and the receivers by synthesizing novel materials.

1.3 Motivation for Relay-Assisted MC Model:

In diffusion-based MC, without any additional infrastructure or external energy, the molecules carrying the information propagate via Brownian motion in all available directions in a fluidic medium. A major challenge in diffusion-based MC is posed by the very limited range of the communication due to the attenuation of molecular signal over distance and also due to diffusion. Characterization of the physical channel of diffusion-based MC in literature shows that the amplitude of a received molecular pulse (i.e., the concentration of information molecules) is inversely proportional to the third power of the transmission distance. For this reason, noticeable performance degradation is observed when the transmission distance increases [11]. One promising solution for overcoming this problem is to deploy intermediate nanomachines acting as relays between the transmitter and its intended receiver nanomachine. There exist several research efforts about relay-assisted molecular communication in the literature.

In literature [12], a relaying scheme is introduced in a diffusion-based MC system based on the enhanced transmission model and it is shown that the relaying scheme will bring significant benefits to the communication reliability. In this project, a diffusion-based MC system with flow assisted propagation and an intermediate nanomachine acting as a relay for improving the reliability of message transmission over long distances is considered and then, the performance of the proposed system is evaluated by studying the optimal detection problem at the receiver end and analyzing the impact of different parameters on the performance of the system. The derived results are plotted in MATLAB to verify them.

The relay-assisted molecular communication system proposed in this report is, in general, a diffusion based molecular communication.

1.4 Potential Applications

There are many potential applications for MC at microscales, such as medical application, control and detection of chemical reactions, computational biology, better understanding of biology, environmental control and preservation, and communication among nanorobots. The main driving force for engineering MC is the medical field with applications in lab-on-a-chip devices, cell-on-chips devices, point-of-care diagnostic chips, and targeted drug delivery. In many of these applications, communication between different components or devices is the key to unlocking their true potential.

One of the main applications envisioned in medicine is artificial immune system. In this case, tiny artificial devices are injected into the body, where each device is specialized for a specific task. For example, one device can be specialized to find pathogens, while another is tasked with destroying the pathogens. This is very similar to the immune system, where each immune cell type carries a specific task. Just like the immune system, to function collectively, these devices need to communicate and collaborate with each other. Taking cues from nature, the most promising solution to solving this communication problem would be MC.

Another driving force behind MC is recent advancements in the field of nanotechnology, which is making nanoscale devices such as nanorobots a reality. Limited by their size, nanorobots can perform only simple tasks. Communication and cooperation among nanorobots can result in performing complex tasks. Communicating nanorobots can be used for biomedical engineering applications, where nanorobots inside the body provide significant improvements in diagnosis and treatment of diseases. In [13], it is shown that communicating nanorobots can be much more effective at targeted drug delivery than uncommunicative nanorobots. In [14], nanorobots are proposed for detection of brain aneurysm. Nanorobots can also be used for transporting molecular payloads to cells, and altering the cell's behavior. In [15], pharmacokinetics of targeted drug delivery systems is analytically modeled through the abstraction of MC. Based on this model, the biodistribution at the target location is estimated with the help of concepts from communication engineering, such as channel delay, path loss,

and the drug accumulation in the rest of the body. Also a procedure to optimize the drug injection rate is proposed that is based on the derived models.

Thus, the applications in which molecular communication can be used are innumerous and so, this field of study is advancing with a great pace.

1.5 Objectives

The main objective of this project is to achieve a reliable wireless molecular communication model at microscale. The reliability depends on the accuracy of the communication, meaning how accurately the information sent from the transmitter is detected by the receiver. In virtue of this, the main objective is divided into two parts:

a. **Derivation**: To derive end-to-end error probability for the proposed relay-assisted molecular communication system.
b. **Optimization and Analysis**: Propose and obtain solution for the optimization problem with respect to threshold detection at end receiver node to minimize the end-to-end error probability. Analyze the impact of different parameters - that monitor the error probability - on the performance of the system. Introduce the joint optimization problem.

Chapter 2

Design and Derivation

After getting a brief understanding about a molecular communication model, this chapter introduces the selected features of the model which will generate parameters on which the end-to-end error probability depends. The introduction to these features is followed by a detailed description of the proposed model in 1D environment and the method by which the end-to-end error probability is derived.

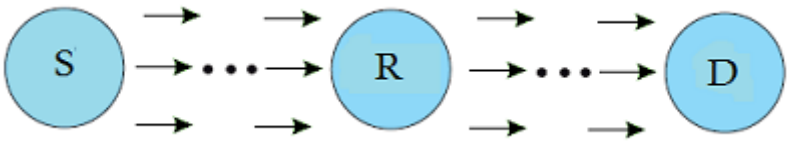
2.1 Unique Features of the Relay-Assisted MC model:

- **Transmitters and receivers of finite size -** Even though the scale in which this molecular communication takes place is in nano or micro, the fact that size of source and receiver can be comparable to the distance between these components cannot be neglected as it would change the solution to the laws of diffusion and thus, change the error probability expression. Therefore, the proportion of the radius of source, relay and destination as shown in Fig. 2.1 with respect to the distance between these micromachines will play an important role in determining the error probability. Moreover, this aspect also serves to make the system more practical because in reality the molecules will have definite size and would not be point source with respect to other quantities like distance between molecules or distance between source and receiver. In this report, the impact of the proportion of radius of machines in 1D medium to the distance between them is analyzed.
- **Fluid medium with positive drift** - A positive drift of the medium that is from transmitter to receiver is considered in addition to the diffusion process. As diffusion process can be slow due to random motion of the molecules in the medium, fluid with positive drift will provide the molecules a direction towards the receiver which will assist them to reach the receiver in less time with accuracy and thus, reduce the performance degradation of the system. An application where a positive drift from transmitter to receiver is present is a healthcare application inside one of the blood vessels. An example of numerous healthcare applications of MC system is in the detection and monitoring cholesterol or disease

precursors in the blood vessels. In this report, the effect of drift velocity on the performance of the system is analyzed.

- **Molecules with finite life expectancy** – Molecular degradation is considered over time, since sometimes the molecules may undergo physical changes or deform over time due to the presence of other molecules or chemicals, or due to change in the pH value of the fluid. It is natural of molecules to degrade and so considering it in the model is more practical. The effect of molecular degradation over error probability is analyzed in this report.
- **All types of noises considered** - The received symbol is corrupted by interference from the previous symbols as well as other noise sources present in the medium. Thus, different types of noises include Inter Symbol Interference (ISI) which refers to the stray molecules from previous symbol durations that arrive in the current symbol duration. ISI from more than one previous durations is considered in this project to completely take ISI in effect. Other noises considered are counting noise and noises from other random sources. The counting noise N_c is defined as the error in counting the molecules at the receiver which are counted by a counter at the receiver. The counting noise is a zero mean process and its variance is dependent on the expected or mean number of molecules received in the current slot. The consideration of different noises present in the environment make the system more compatible to noises and more reliable.
- **Relay assisted transmission considered** - The existence of an intermediate nanomachine acting as a relay for improving the reliability of message transmission between the transmitter and receiver. The use of relaying can be substantiated by its use in different biological processes such as transferring the DNA sequences from bacteria to bacteria using bacterial conjugation, a process that involves transfer of single stranded DNA from one cell to another or use of artificial cells as relay nodes to detect the intended message and decode it to send a message to Escherichia Coli (E. Coli) cells. It is analyzed in this report that relaying provides significant communication reliability.

2.2 Relay-Assisted Molecular Communication Model with Line Micromachines



Source of radius r_S | Relay of radius r_R | Destination of radius r_D

Fig. 2.1: Relay-assisted MC model in 1D environment.

The diffusion based relay-assisted molecular communication model comprises of a line source (transmitter) and a line destination (receiver) with an additional line relay node - which is a source as well as a receiver - having a finite radius r_S, r_D and r_R respectively. These elements are suspended in a 1D fluid environment having diffusion coefficient D. The elements, thus, have a linear volume of $2r_S$, $2r_D$ and $2r_R$ respectively. The center of the source is at origin. The distance between the centers of source and relay is denoted by d_{SR} and that between the centers of relay and destination is denoted by d_{RD}. Since the receivers i.e. relay and destination are of perfectly absorbing type and the absorption takes place at the surface of the receivers, the effective distance between the source and relay is $d_1 = d_{SR} - r_R$ and that between the relay and destination is $d_2 = d_{RD} - r_D$. All the elements are synchronized with time. The channel is divided into different time slots of duration T, where the j^{th} slot is defined as the time period [(j − 1)T, jT), with j ϵ {1, 2, . . .}. In this communication, it is considered that binary information is sent which comprises of bit 1 and bit 0. The apriori probability of sending bit 1 or bit 0 is assumed to be equal to 0.5 each.

2.2.1 Diffusion Process between Source and Relay in k^{th} Slot.

Starting at t = 0, the transmitter emits a fixed number of molecules at the beginning of every slot. The emission process is controlled by a stimulus given to the transmitter. We assume that the transmitter can accurately control the number of molecules emitted. According to the binary amplitude modulation scheme (concentration shift keying), the transmitter releases N_{Ax}

molecules at the starting of every symbol duration for sending bit x where N_{Ax}=N_A for x=1 and N_{Ax}=0 for x=0.

The emitted molecules after being released are free to diffuse in all directions in the medium with drift. While propagating through the medium, the molecules follow Brownian motion with a net drift from the transmitter to the receiver. The motion is determined by two parameters of the fluid medium: the drift velocity v and the diffusion coefficient D. Brownian motion of molecules is modeled as a Wiener process [21] with variance σ^2 = 2D. An increment in the position of a molecule over a time interval (t_1, t_2) has a Gaussian distribution with mean v($t_1 - t_2$) and variance σ^2 ($t_1 - t_2$), and these increments are independent of each other for non-overlapping time intervals.

Initially considering the source to be a point source and the relay acting as a perfectly absorbing surface, we will find the probability with which a molecule sent from the point source reach the surface of the relay at x = d_1 over a symbol duration T.

Firstly, the first arrival time t of the molecule from a point source for a fixed displacement x = d_1 is of prime importance. The first arrival time follows an inverse Gaussian distribution with a probability density function (PDF) given by

$$g(t) = \sqrt{\frac{\lambda}{2\pi t^3}}.\exp\left(-\frac{\lambda(t-\mu)^2}{2\mu^2 t}\right), \quad \text{for t>0} \quad \text{where } \mu = d_1/v \text{ and } \lambda = {d_1}^2/\sigma^2$$

$$\therefore g(t) = \left(\frac{d_1}{\sqrt{4\pi D t^3}}\right).\exp\left(\frac{-(d_1 - vt)^2}{4Dt}\right), \quad \text{for t > 0}$$

This equation gives the probability that a molecule will reach the relay at d_1 from a point source at any time t > 0. The derivation of this probability is provided in literature [16].

Furthermore, molecular degradation is considered due to which the molecules have some life expectancy that can modeled as an exponential distribution whose PDF is given by

$$h(\tau) = \alpha.\exp(-\alpha\tau), \ \tau > 0$$

Here α is referred to as the degradation parameter and τ represents the lifetime of molecules. The relation between half-life of a molecule and the molecular degradation coefficient is inversely proportional and is given in literature [17] as $\alpha = \ln 2/\lambda_{1/2}$ where $\lambda_{1/2}$ denotes the half-life of the molecules. A molecule can reach the receiver in time t only if its lifetime is more than t, i.e. $\tau \in (t, \infty)$. Molecules failing to reach in the current slot 'k' remain in the medium and appear as stray molecules in the subsequent slots.

Let p_i denote the probability that a molecule transmitted in the i^{th} previous slot arrives in the current slot k, and is given by

$$p_i = \int_{iT}^{(i+1)T} g(t) \int_{t}^{\infty} h(\tau)\, d\tau dt = \int_{iT}^{(i+1)T} g(t) \exp(-\alpha t)\, dt$$

where i is an integer and $i \in [1, L]$ where L is the ISI length.

The probability (CDF) of successful arrival of a molecule over time slot iT starting from t=0 in the current slot is given by f_i.

$$f_i = \int_{0}^{iT} g(t).\exp(-\alpha t)\, dt$$

The probability of successful arrival of a molecule over time T of the current symbol duration is given by f_0. In other words, f_0 gives the probability with which a molecule released in the current slot will reach the relay in the current slot.

$$f_0 = \int_{0}^{T} g(t).\exp(-\alpha t)\, dt$$

$$f_0 = \exp\left(\frac{d_1(v - v')}{2D}\right)\left\{1 + \frac{1}{2}\left[\exp\left(\frac{vd_1}{D}\right) erfc\left(\frac{vT + d_1}{\sqrt{4DT}}\right) - erf\left(\frac{vT - d_1}{\sqrt{4DT}}\right)\right]\right\}$$

Here, erf is an error function. Refer to Appendix A for its definition and properties.

$$v' = \sqrt{v^2 + 4D\alpha}$$

$$p_i = \int_0^{(i+1)T} g(t).\exp(-\alpha t)\,dt - \int_0^{iT} g(t).\exp(-\alpha t)\,dt$$

The above derived probabilities are with respect to point source. Now, the probabilities for a volume source can be derived by taking mean of the earlier probabilities over the total volume of the source [18]. Thus, the probability of successful arrival for a molecule transmitted in the current slot is given by $f_0|_{V_S}$.

$$f_0|_{V_S} = \frac{1}{|V_S|}\int_{V_S} f_0 dV_S$$

$$\therefore f_0|_{V_S} = \frac{1}{2r_S}\int_{-2r_S}^{2r_S} f_0 dc$$

where c is the distance from the center of the transmitter to an arbitrary point in V_S.

If we define the vectors $\overrightarrow{r_c}$ and $\overrightarrow{r_d}$ relative to the center of the transmitter, such that $\overrightarrow{r_c}$ = c and $\overrightarrow{r_d}$ = d_1 (i.e., $\overrightarrow{r_d}$ is the vector from the center of the transmitter to the center of the receiver), then the distance from the center of the receiver to an arbitrary point in V_S, $d_{int} = |\overrightarrow{r_c} - \overrightarrow{r_d}|$ = d_1 + c. The above integral is solved by substituting d_1 as d_{int} and the final expression is obtained as follows:

$$f_0|_{V_S} = \frac{1}{4r_S}\left\{\begin{aligned}
&\left(\frac{2D}{v+v'}\right)\left[\exp\left(\frac{(v+v')(d_1+r_S)}{2D}\right).erfc\left(\frac{v'T+d_1+r_S}{\sqrt{4DT}}\right) - \exp\left(\frac{(v+v')(d_1-r_S)}{2D}\right).erfc\left(\frac{v'T+d_1-r_S}{\sqrt{4DT}}\right)\right] \\
&-\left(\frac{2D}{v-v'}\right)\left[\exp\left(\frac{(v-v')(d_1+r_S)}{2D}\right).erfc\left(\frac{v'T-d_1-r_S}{\sqrt{4DT}}\right) - \exp\left(\frac{(v-v')(d_1-r_S)}{2D}\right).erfc\left(\frac{v'T-d_1+r_S}{\sqrt{4DT}}\right)\right] \\
&+\left(\frac{4Dv}{v^2-v'^2}\right)\exp\left(\frac{(v^2-v'^2)T}{4D}\right)\left[erfc\left(\frac{vT-d_1+r_S}{\sqrt{4DT}}\right) - erfc\left(\frac{vT-d_1-r_S}{\sqrt{4DT}}\right)\right] \\
&+\left(\frac{4D}{v-v'}\right)\left[\exp\left(\frac{(v-v')(d_1+r_S)}{2D}\right) - \exp\left(\frac{(v-v')(d_1-r_S)}{2D}\right)\right]
\end{aligned}\right\}$$

Similarly, other probabilities will be derived by solving the following integrals:

$$p_i|_{V_S} = \frac{1}{2r_S}\int_{-2r_S}^{2r_S}\left(f_{i+1} - f_i\right)dc$$

Now, for k^{th} slot, let Q_A represent the number of molecules received from the current slot k, I_{Ai} represent the number of stray molecules arriving in the current slot from the i^{th} previous slot, N_{Ao} denotes the number of molecules received from other random sources and N_{Ac} represent the counting noise. The distributions of Q_A and I_{Ai} are approximated to be Gaussian for large N_A and the quantities N_{Ao} and N_{Ac} are assumed to be Gaussian random variables.

$$Q_A \sim N\left(\mu_{Q_A} = N_{Ax}.f_0|_{V_S},\ \sigma^2_{Q_A} = N_{Ax}.\ f_0|_{V_S}(1\text{-}f_0|_{V_S})\right)$$

$$I_{Ai} \sim N\left(\mu_{I_{Ai}} = {}^{N}{}_{Ax}.p_i|_{V_S}, \sigma^2_{I_{Ai}} = {}^{N}{}_{Ax}.p_i|_{V_S}\left(1 - p_i|_{V_S}\right)\right)$$

To make the interference of molecules from previous slots independent of the transmitted symbol x, average is taken over all possible transmissions to obtain the mean μ_{Ii} and variance σ^2_{Ii} as

$\mu_{I_{Ai}} = \sum_{x=0}^{1} a_x \mu_{I_{Aix}}$ where $\mu_{I_{Aix}} = N_{Ax}.\ p_i|_{V_S}$ and a_x is the apriori probability which is 0.5 for x=0 and x=1 both.

$$\mu_{I_{Ai}} = \frac{{}^{N}{}_{A}.p_i|_{V_S}}{2}$$

$$\sigma^2_{I_{Ai}} = E\left[I^2_{Ai}\right] - \mu^2_{I_{Ai}}$$

$$E\left[I^2_{Ai}\right] = \sum_{x=0}^{1} a_x\left(N^2_{Ax}.\left(p_i|_{V_S}\right)^2 + {}^{N}{}_{Ax}.p_i|_{V_S}\cdot\left(1 - p_i|_{V_S}\right)\right)$$

$$\therefore E\left[I^2_{Ai}\right] = a_1\left(N^2_{Ax}.\left(p_i|_{V_S}\right)^2 + {}^{N}{}_{Ax}.p_i|_{V_S}\cdot\left(1 - p_i|_{V_S}\right)\right)$$

$$\sigma^2_{I_{Ai}} = a_1 {}^{N}{}_{A}.p_i|_{V_S}\cdot\left(1 - p_i|_{V_S}\right) + a_1.a_0 N^2_{A}.\left(p_i|_{V_S}\right)^2$$

$$\therefore \sigma^2_{I_{Ai}} = \frac{N_A.p_i\,|_{V_S}\cdot\left(1-p_i\,|_{V_S}\right)}{2} + \frac{N_A^2.\left(p_i\,|_{V_S}\right)^2}{4}$$

Finally, the distribution of other noise sources is as follows:

$$N_{Ac} \sim N\,(\mu_{N_{Ac}} = 0,\ \sigma^2_{Ax}) \text{ and } N_{Ao} \sim N\,(\mu_{N_{Ao}},\ \sigma^2_{N_{Ao}})$$

Ultimately, the total number of molecules received in the k^{th} slot is given by the random variable A_x which will also have Gaussian distribution with parameters μ_{Ax} and σ^2_{Ax}, since it is the sum of Gaussian random variables. Since all the transmissions are considered to be independent of each other, the mean and variance of R_x are obtained as:

$$\mu_{Ax} = \mu_{Q_A} + \sum_{i=1}^{L}\mu_{I_{Ai}} + \mu_{N_{Ac}} + \mu_{N_{Ao}} \text{ and } \sigma^2_{Ax} = \sigma^2_{Q_A} + \sum_{i=1}^{L}\sigma^2_{I_{Ai}} + \sigma^2_{N_{Ac}} + \sigma^2_{N_{Ao}}$$

Now, since the apriori probability for x=0 and x=1 is equal, Maximum Likelihood-ratio (ML) test is used to derive the detection threshold τ_R at the relay node.

$$\frac{\Pr\left(A_x \mid x_k = 0\right)}{\Pr\left(A_x \mid x_k = 1\right)} = 1$$

$$\therefore \frac{1}{\sqrt{2\pi\sigma^2_{A0}}}\exp\left(-\frac{\left(\tau_R-\mu_{A0}\right)^2}{2\sigma^2_{A0}}\right) = \frac{1}{\sqrt{2\pi\sigma^2_{A1}}}\exp\left(-\frac{\left(\tau_R-\mu_{A1}\right)^2}{2\sigma^2_{A1}}\right)$$

Solving the above expression for τ_R gives

$$\tau_R = \text{round}\left(\frac{\left(\sqrt{B^2+2A\ln C}\right)-B}{A}\right)$$

where $A = \frac{\sigma^2_{A1}-\sigma^2_{A0}}{\sigma^2_{A1}.\sigma^2_{A0}}$, $B = \frac{\sigma^2_{A0}\mu_{A1}-\sigma^2_{A1}\mu_{A0}}{\sigma^2_{A1}.\sigma^2_{A0}}$, $C = \left(\frac{\sigma_{A0}}{\sigma_{A1}}\right).\exp\left(\frac{\mu^2_{A1}}{2\sigma^2_{A1}}-\frac{\mu^2_{A0}}{2\sigma^2_{A0}}\right)$.

The detection threshold at the relay node τ_R is the threshold number of molecules which helps the relay in deciding the information sent by the source. If the number of molecules counted by the relay or receiver is lesser than the threshold value τ_R, relay will decide that bit 0 was

sent. On the other hand, if the number of molecules counted by the relay are greater than the threshold value, the relay will decide that bit 1 was sent. Thus, the diffusion process between source and relay ends by decoding the information present in the molecules and detecting whether bit 1 or bit 0 was sent.

2.2.2 Diffusion Process between Relay and Destination in $(\mathrm{k}+1)^{th}$ Slot

The relay receives the molecules released in the k^{th} **slot** by the source. The relay decodes the information encoded in these molecules, makes a decision on the basis of ML criteria at the end of the current slot and then again encodes the information in molecules and release them at the start of the next slot $(\boldsymbol{k+1})^{th}$ slot. The slot is k+1 with respect to the source. The destination node collects the molecules and decodes the information at the end of the $(\boldsymbol{k+1})^{th}$ slot. The relay, according to the binary concentration shift keying, releases N_{Bx} molecules at the starting of every symbol duration for sending bit x where N_{Bx}=N_B for x=1 and N_{Bx}=0 for x=0.

The method to derive the probability that a molecule transmitted in the i^{th} previous slot arrives in the current slot will be same as discussed earlier in the chapter diffusion process between source and relay in the k^{th} slot except that some variables will change such as the radius of source will be replaced by the radius of the relay and the effective distance between source and relay will be replaced by the effective distance between relay and destination.

Thus, the probability of successful arrival of a molecule transmitted by a point source (relay) in the current slot k+1 is given by

$$f_0 = \exp\left(\frac{d_2\left(v-v^{'}\right)}{2D}\right)\left\{1+\frac{1}{2}\left[\exp\left(\frac{vd_2}{D}\right)erfc\left(\frac{vT+d_2}{\sqrt{4DT}}\right)-erf\left(\frac{vT-d_2}{\sqrt{4DT}}\right)\right]\right\}$$

The probability of successful arrival of a molecule in the current slot which is transmitted by the relay of finite linear volume is given by $f_0|_{V_R}$.

$$f_0|_{V_R} = \frac{1}{4r_R}\left\{\begin{array}{l}\left(\frac{2D}{v+v'}\right)\left[\exp\left(\frac{(v+v')(d_2+r_R)}{2D}\right).erfc\left(\frac{v'T+d_2+r_R}{\sqrt{4DT}}\right)-\exp\left(\frac{(v+v')(d_2-r_R)}{2D}\right).erfc\left(\frac{v'T+d_2-r_R}{\sqrt{4DT}}\right)\right] \\ -\left(\frac{2D}{v-v'}\right)\left[\exp\left(\frac{(v-v')(d_2+r_R)}{2D}\right).erfc\left(\frac{v'T-d_2-r_R}{\sqrt{4DT}}\right)-\exp\left(\frac{(v-v')(d_2-r_R)}{2D}\right).erfc\left(\frac{v'T-d_2+r_R}{\sqrt{4DT}}\right)\right] \\ +\left(\frac{4Dv}{v^2-v'^2}\right)\exp\left(\frac{(v^2-v'^2)T}{4D}\right)\left[erfc\left(\frac{vT-d_2+r_R}{\sqrt{4DT}}\right)-erfc\left(\frac{vT-d_2-r_R}{\sqrt{4DT}}\right)\right] \\ +\left(\frac{4D}{v-v'}\right)\left[\exp\left(\frac{(v-v')(d_2+r_R)}{2D}\right)-\exp\left(\frac{(v-v')(d_2-r_R)}{2D}\right)\right]\end{array}\right\}$$

Similarly, the probability that a molecule transmitted by the relay of finite volume in the i^{th} previous slot arrives in the current slot will be given by $p_i|_{V_R}$.

$$p_i|_{V_R} = \frac{1}{2r_R}\int_{-2r_R}^{2r_R}\left(f_{i+1}-f_i\right)dc$$

where i is an integer and i ϵ [1, L] where L is the ISI length and where c is the distance from the center of the relay to an arbitrary point in V_R.

Now, for $k+1^{th}$ slot, let Q_B represent the number of molecules received in the current slot k+1, I_{Bi} represent the number of stray molecules arriving in the current slot from the i^{th} previous slot, N_{Bo} denotes the number of molecules received from other random sources and N_{Bc} represent the counting noise. The distributions of Q_B and I_{Bi} are approximated to be Gaussian for large N_A and the quantities N_{Ao} and N_{Ac} are assumed to be Gaussian random variables.

$$Q_B \sim N\left(\mu_{Q_B} = N_{Bx}.f_0|_{V_R},\ \sigma^2_{Q_B} = N_{Bx}.f_0|_{V_R}(1-f_0|_{V_R})\right)$$

$$I_{Bi} \sim N\left(\mu_{I_{Bi}} = N_{Bx}.p_i|_{V_S},\ \sigma^2_{I_{Bi}} = N_{Bx}.p_i|_{V_R}\left(1-p_i|_{V_R}\right)\right)$$

To make the interference of molecules from previous slots independent of the transmitted symbol x, average is taken over all possible transmissions to obtain the mean μ_{Ii} and variance σ^2_{Ii} as

$\mu_{I_{Bi}} = \sum_{x=0}^{1} b_x \mu_{I_{Bix}}$ where $\mu_{I_{Bix}} = N_{Bx}.\ p_i\,|_{V_R}$ and b_x is the apriori probability. Refer appendix C for apriori probabilities (b_0 and b_1).

$$\mu_{I_{Bi}} = \frac{N_B . p_i\,|_{V_R}}{2}$$

$$\sigma^2_{I_{Bi}} = E\left[I^2_{Bi}\right] - \mu^2_{I_{Bi}}$$

$$E\left[I^2_{Bi}\right] = \sum_{x=0}^{1} b_x \left(N^2_{Bx} . \left(p_i\,|_{V_R}\right)^2 + N_{Bx} . p_i\,|_{V_R} . \left(1 - p_i\,|_{V_R}\right)\right)$$

$$\therefore E\left[I^2_{Bi}\right] = b_1 \left(N^2_{Bx} . \left(p_i\,|_{V_R}\right)^2 + N_{Bx} . p_i\,|_{V_R} . \left(1 - p_i\,|_{V_R}\right)\right)$$

$$\sigma^2_{I_{Bi}} = b_1 N_B . p_i\,|_{V_R} . \left(1 - p_i\,|_{V_R}\right) + b_1 . b_0 N^2_B . \left(p_i\,|_{V_R}\right)^2$$

$$\therefore \sigma^2_{I_{Bi}} = \frac{N_B . p_i\,|_{V_R} . \left(1 - p_i\,|_{V_R}\right)}{2} + \frac{N^2_B . \left(p_i\,|_{V_R}\right)^2}{4}$$

Finally, the distribution of other noise sources is as follows:

$$N_{Bc} \sim N\left(\mu_{N_{Bc}} = 0, \sigma^2_{N_{Bx}}\right) \text{ and } N_{Ao} \sim N\left(\mu_{N_{Bo}}, \sigma^2_{N_{Bo}}\right)$$

Ultimately, the total number of molecules received in the k^{th} slot is given by the random variable A_x which will also have Gaussian distribution with parameters μ_{Bx} and σ^2_{Bx}, since it is the sum of Gaussian random variables. Since all the transmissions are considered to be independent of each other, the mean and variance of R_x are obtained as:

$$\mu_{Bx} = \mu_{Q_{Bk}} + \sum_{i=1}^{L} \mu_{I_{Bi}} + \mu_{N_{Bc}} + \mu_{N_{Bo}} \text{ and } \sigma^2_{Bx} = \sigma^2_{Q_{Bk}} + \sum_{i=1}^{L} \sigma^2_{I_{Bi}} + \sigma^2_{N_{Bc}} + \sigma^2_{N_{Bo}}$$

Finally, deriving a term for end to end error probability for the k^{th} bit is given by $P_e[k]$.

$$P_e[k] = \Pr\left(x_{S(k)} = 1\right).\Pr\left(x_{D(k+1)} = 0 \mid x_{S(k)} = 1\right) + \Pr\left(x_{S(k)} = 0\right).\Pr\left(x_{D(k+1)} = 1 \mid x_{S(k)} = 0\right)$$

$$\Pr\left(x_{D(k+1)} = 0 \mid x_{S(k)} = 1\right) = \begin{bmatrix} \Pr\left(x_{R(k+1)} = 0 \mid x_{S(k)} = 1\right).\Pr\left(x_{D(k+1)} = 0 \mid x_{S(k)} = 1\right) \\ + \Pr\left(x_{R(k+1)} = 1 \mid x_{S(k)} = 1\right).\Pr\left(x_{D(k+1)} = 0 \mid x_{S(k)} = 1\right) \end{bmatrix}$$

$x_{S(k)}$ represents the bit sent by source at k^{th}, $x_{R(k+1)}$ represents the bit sent by relay at $k+1^{th}$slot, and $x_{D(k+1)}$ represents the bit detected by the destination in $k+1^{th}$slot.

$$\Pr(x_{D(k+1)}=0 \mid x_{S(k)}=1) = \left[1-Q\left(\frac{\tau_R-\mu_{A1}}{\sigma_{A1}}\right)\right].\left[1-Q\left(\frac{\tau_D-\mu_{B0}}{\sigma_{B0}}\right)\right] + Q\left(\frac{\tau_R-\mu_{A1}}{\sigma_{A1}}\right).\left[1-Q\left(\frac{\tau_D-\mu_{B1}}{\sigma_{B1}}\right)\right]$$

$$\Pr(x_{D(k+1)}=0 \mid x_{S(k)}=1) = \left\{\begin{array}{l}\frac{1}{2}\left[1+\text{erf}\left(\frac{\tau_R-\mu_{A1}}{\sqrt{2\sigma_{A1}^2}}\right)\right].\frac{1}{2}\left[1+\text{erf}\left(\frac{\tau_D-\mu_{B0}}{\sqrt{2\sigma_{B0}^2}}\right)\right] \\ +\ \frac{1}{2}\left[1-\text{erf}\left(\frac{\tau_R-\mu_{A1}}{\sqrt{2\sigma_{A1}^2}}\right)\right].\frac{1}{2}\left[1+\text{erf}\left(\frac{\tau_D-\mu_{B1}}{\sqrt{2\sigma_{B1}^2}}\right)\right]\end{array}\right\}$$

Similarly,

$$\Pr(x_{D(k+1)}=1 \mid x_{S(k)}=0) = \left[1-Q\left(\frac{\tau_R-\mu_{A0}}{\sigma_{A0}}\right)\right].\left[1-Q\left(\frac{\tau_D-\mu_{B0}}{\sigma_{B0}}\right)\right] + Q\left(\frac{\tau_R-\mu_{A0}}{\sigma_{A0}}\right).\left[1-Q\left(\frac{\tau_D-\mu_{B1}}{\sigma_{B1}}\right)\right]$$

$$\Pr(x_{D(k+1)}=1 \mid x_{S(k)}=0) = \left\{\begin{array}{l}\frac{1}{2}\left[1+\text{erf}\left(\frac{\tau_R-\mu_{A0}}{\sqrt{2\sigma_{A0}^2}}\right)\right].\frac{1}{2}\left[1-\text{erf}\left(\frac{\tau_D-\mu_{B0}}{\sqrt{2\sigma_{B0}^2}}\right)\right] \\ +\ \frac{1}{2}\left[1-\text{erf}\left(\frac{\tau_R-\mu_{A0}}{\sqrt{2\sigma_{A0}^2}}\right)\right].\frac{1}{2}\left[1-\text{erf}\left(\frac{\tau_D-\mu_{B1}}{\sqrt{2\sigma_{B1}^2}}\right)\right]\end{array}\right\}$$

$$\Pr(x_{S(k)}=0) = \Pr(x_{S(k)}=1) = 0.5$$

$$\therefore P_e[k] = 0.5+0.125\left[erf\left(\frac{\tau_R-\mu_{A1}}{\sqrt{2\sigma_{A1}^2}}\right)-erf\left(\frac{\tau_R-\mu_{A0}}{\sqrt{2\sigma_{A0}^2}}\right)\right].\left[erf\left(\frac{\tau_D-\mu_{B0}}{\sqrt{2\sigma_{B0}^2}}\right)-erf\left(\frac{\tau_D-\mu_{B1}}{\sqrt{2\sigma_{B1}^2}}\right)\right]$$

This is the end to end error probability which is function of τ_D i.e. detection threshold at destination. The detection threshold at the destination node is not calculated is not evaluated using MAP criteria, rather is treated as a variable because this threshold value will not just depend on the diffusion process between relay and destination. It should be evaluated on the basis of the whole diffusion process between source and destination. Moreover, the evaluated threshold at destination $\tau_D$should be such that the error probability $P_e[k]$ is minimum at τ_D. So, to avoid any inaccuracy in measuring the threshold value, it is treated as a variable and an optimization problem is formulated so as to get the desired minimum error probability.

Chapter 3

Error Performance Optimization

In the last chapter, the end-to-end error probability was derived as a function of threshold detection at destination node (τ_D). In this chapter, the optimization problem with respect to τ_D is proposed and analyzed and accordingly, a solution is implemented. Further the joint optimization problem on two parameters viz. distance of relay from source and molecules allocated to source, is introduced and a 3D plot for the joint optimization problem is plotted to demonstrate the optimal value of the parameters.

3.1 Detection Threshold Optimization Problem:

The objective is to determine the bit error probability of the system which is a function of detection threshold at destination (τ_D). Therefore, to find the optimal detection threshold (τ_D) which yields the minimum bit error probability, the problem is formulated as an optimization problem as follows:

$$\min_{\tau_D} P_e[k] = 0.5+0.125\left[erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) - erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) \right].\left[erf\left(\frac{\tau_D - \mu_{B0}}{\sqrt{2\sigma_{B0}^2}} \right) - erf\left(\frac{\tau_D - \mu_{B1}}{\sqrt{2\sigma_{B1}^2}} \right) \right]$$

In order to verify the convexity (or concavity) of the above optimization problem with no constraint, the second derivative of the objective function is needed. Thus, the second derivative of $P_e[k]$ with respect to the optimization variable (τ_D) is given by:

$$\frac{d^2}{d\tau_D^2} P_e[k] = g.\left[\left(-\sqrt{\frac{2}{\pi}} \right) \left(\frac{\tau_D - \mu_{B0}}{\sigma_{B0}^3} \right) \exp\left(-\left(\frac{\tau_D - \mu_{B0}}{\sqrt{2\sigma_{B0}^2}} \right)^2 \right) + \left(\sqrt{\frac{2}{\pi}} \right) \left(\frac{\tau_D - \mu_{B1}}{\sigma_{B1}^3} \right) \exp\left(-\left(\frac{\tau_D - \mu_{B1}}{\sqrt{2\sigma_{B1}^2}} \right)^2 \right) \right]$$

$$\text{where } g = 0.125\left[erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) - erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) \right]$$

It can be observed that the second derivative of the objective function $P_e[k]$ is positive for some value of the optimization variable (τ_D) and negative for some other value of the variable. For instance, if $\tau_D > \mu_{B0}$ and $\tau_D < \mu_{B1}$, the second derivative will be negative. On the other hand, if $\tau_D < \mu_{B0}$ and $\tau_D > \mu_{B1}$, the second derivative will be positive. Hence, the optimization problem is not convex. In the next section, the method to solve this optimization problem using MATLAB is proposed.

3.2 Solution to the Optimization Problem:

Since, the problem is concave for some value of threshold and convex for some other value of threshold, it cannot be solved by simply taking the second derivative of the objective function as seen in the above section. Thus, this problem is solved in MATLAB using a function that optimizes a non-linear function of a constrained variable. This function is available in the optimization toolbox of MATLAB and uses some mathematical methods to solve the optimization problem.

The proposed code to solve the optimization problem involves using the function fminbnd(), in which one needs to pass the function and the constrained interval of the optimization variable in which the objective function should be the minimum. 'fminbnd' is a one-dimensional minimizer that finds a minimum for a problem specified by $\min_x f(x)$ such that $x_1 < x < x_2$ where x_1, x, x_2 are finite scalars, and f(x) is a function that returns a scalar.

In the proposed optimization problem, the constrained interval for τ_D is (μ_{B0}, μ_{B1}). As the threshold value should be between the expected or mean number of values expected for bit 0 and mean number of values expected for bit 1. Thus, the code to solve the optimization problem comprises of code to define the function $P_e[k]$ as a function of τ_D and then, find the optimized value th_optim such that th_optim = fminbnd($P_e[k]$, μ_{B0}, μ_{B1}).

To see the results of theoretical value with the observed value, numerical results are illustrated in the following sections.

3.3 Numerical Results:

3.3.1 Values Assigned to Different Parameters:

The parameters which determine a change in the end-to-end bit error probability are assigned particular values for the sake of obtaining numerical results. These values are referred from a published research paper [2]. The value of the molecular degradation coefficient are evaluated from the half-life values of molecules from the literature [17]. The values assigned to these parameters is tabulated in the table 3.1.

Parameters	**Variable**	**Values**
Diffusion coefficient	D	242 μm^2/s
Drift velocity	V	[0.3,1] mm/s
Distance between nodes S and D	d_{SD}	1, 1.5 and 2 µm
Radius of source, relay and destination	r_S, r_R, r_D	[0.1, 1] µm
Symbol duration	T	2, 5 and 7 ms
Number of molecules for sending bit 1	N_A, N_B	[40,1000]
Molecular noise variance	$\sigma^2_{N_{Ao}}$, $\sigma^2_{N_{Bo}}$	20, 40, and 100
Molecular noise mean	$\mu_{N_{Ao}}$, $\mu_{N_{Bo}}$	20, 40 and 100
Molecular degradation coefficient	α	40 and 54 s^{-1}
Probability of sending bit 1 and 0 from source	a_1, a_0	0.5, 0.5
ISI length	I	9

Table 3.1: Values of system parameters.

3.3.2 Analysis of Performance based on Optimization Detection Threshold

- The error probability of the system as a function of the detection threshold for different values of drift velocity, number of allocated molecules to source and relay for sending bit 1, T = 5 ms, α = 54 s^{-1} and d_{SD}= 2 μm is plotted and presented in Fig. 3.1.
- Results in Fig. 3.1 show that the error probability on the detection threshold values is a quasiconvex function because its domain and all its sublevel sets are convex. Refer to appendix B for quasiconvex function.
- The optimized value of detection threshold obtained using fminbnd function matches approximately the observed optimal value from the figure 3.1 for different values of N_A, N_B and drift velocity.
- Also, the figure indicates the impact of the appropriate detection threshold on the performance. At optimized value of detection threshold, the error probability reduces significantly. For instance, at v=0.3 mm/s; N_A=N_B=300, the bit error rate is 1.049 x 10^{-14} at the near optimized value of threshold which is a significantly low value.
- Optimized value of detection threshold depends on number of molecules transmitted as can be observed from the Fig. 3.1 that as the number of molecules allotted for sending bit 1 from source and relay is increased, the value of optimal detection threshold increases i.e. the curve shifts towards right. For instance, for v=0.6 mm/s; N_A=N_B=300, the optimal value as observed from the Fig. 3.1 is 242 while for v=0.6 mm/s; N_A=N_B=400, the optimal values becomes 286. This is appropriate as the increase in N_A, N_B will result in increase in the expected number of values for bit 0 and bit 1 i.e.μ_{A0}, μ_{A1}, μ_{B0}, μ_{B1}.
- It can also be observed from Fig. 3.1 that with increase in drift velocity v for the same number of molecules allocated N_A and N_B, the optimized value of detection threshold remains nearly the same while the error probability reduces i.e. the curve shifts upwards. For instance, v=0.3 mm/s; N_A=N_B=300, the error probability is 1.049 x 10^{-14} while for v=0.6 mm/s; N_A=N_B=300, the error probability is 1.238 x 10^{-22}. This is because high drift velocity will speed up the propagation of molecules towards the receiver. Thus, the probability to detect bit 1 will be more certain. The reason for curve not shifting right significantly is that the threshold value does not depend on the drift velocity.

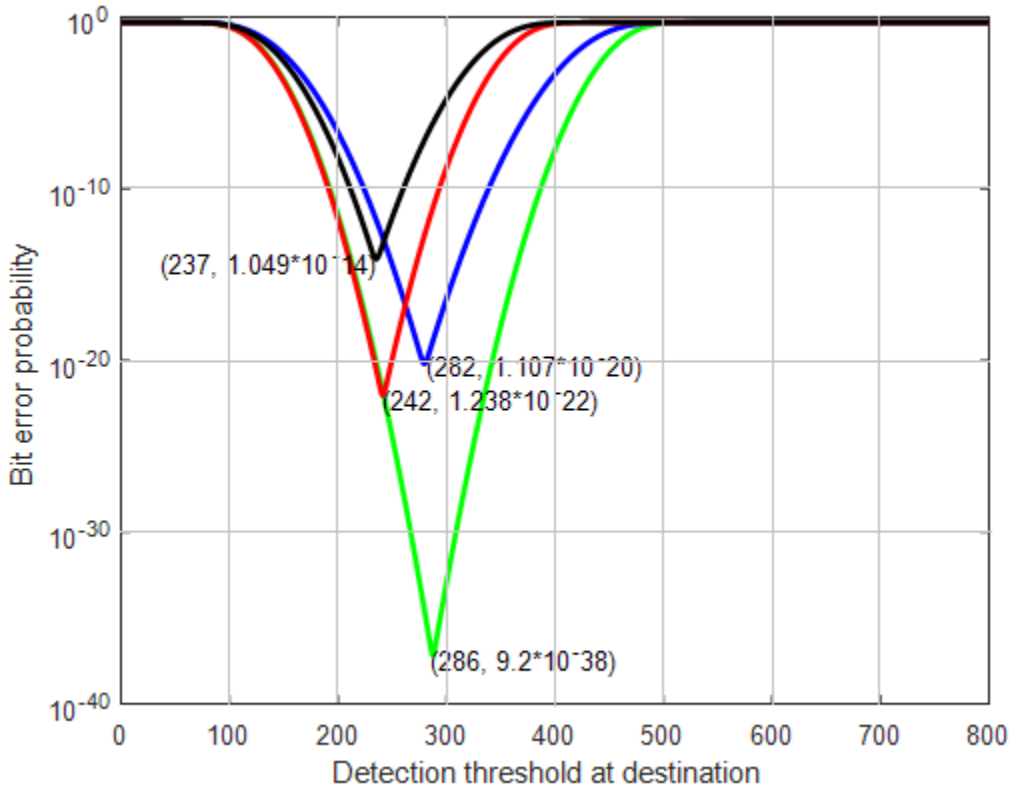


Fig. 3.1: Bit error rate as a function of detection threshold at destination for different values of drift and molecules allocated to source and relay.

Parameters	**Color code**	**Optimal value of detection threshold (τ_D)**
v=0.3 mm/s; N_A=N_B=300	**Black**	**235**
v=0.6 mm/s; N_A=N_B=300	**Red**	**231**
v=0.3 mm/s; N_A=N_B=400	**Blue**	**265**
v=0.6 mm/s; N_A=N_B=400	**Green**	**246**

Table 3.2: Theoretical optimized value of detection threshold at destination for different values of of drift and molecules allocated to source and relay.

3.4 Introduction to Joint Optimization Problem:

In this section the problem of optimizing the performance of the relay-assisted molecular communication system by jointly positioning the relay between the source and the destination and allocating number of molecules to the source is addressed. This type of joint optimization is never addressed in any literature before. In this problem we have two variables defined as:

x: fraction of the distance between source and destination. It is defined as:

$$x = \frac{d_{SR}}{d_{SD}}$$

Therefore, d_{SR} = x. d_{SD} and thus, d_{RD}=(1-x). d_{SD}.

y: fraction of the total number of molecules allocated to source and relay combined (N_T). It is defined as:

$$x = \frac{N_A}{N_B}$$

Therefore, N_A = y. N_T and thus, N_B=(1-y). N_T.

The joint optimization problem is formulated as:

$$\min_{x,y} P_e[k] = 0.5+0.125\left[erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) - erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) \right].\left[erf\left(\frac{\tau_D - \mu_{B0}}{\sqrt{2\sigma_{B0}^2}} \right) - erf\left(\frac{\tau_D - \mu_{B1}}{\sqrt{2\sigma_{B1}^2}} \right) \right]$$

Here, the optimal value of threshold used is the one derived using the solution described in section 3.2. Thus, $P_e[k]$ becomes a function in variables x and y only. Now, the solution to this optimization problem will be easily found if the function in x and y is jointly convex. So, first it is necessary to check whether the function is jointly convex. One way to check the convexity is described in the following section.

3.4.1 Convexity of the Joint Optimization Problem:

As discussed earlier, if the joint optimization problem is convex, then the solution can be derived from second derivatives with respect to only x, only y and x, y both in order and y, x both in order i.e. from $\frac{\partial^2 P_e[k]}{\partial x^2}$, $\frac{\partial^2 P_e[k]}{\partial y^2}$, $\frac{\partial^2 P_e[k]}{\partial x.\partial y}$ and $\frac{\partial^2 P_e[k]}{\partial y.\partial x}$. So, to check the convexity of

the objective function, one solution is to plot a 3D graph of $P_e[k]$ vs. x and y. The graph will denote the points where the function will be convex or concave. If the function has points at which it is concave as well as convex, then the function is not convex. Otherwise, it is completely convex.

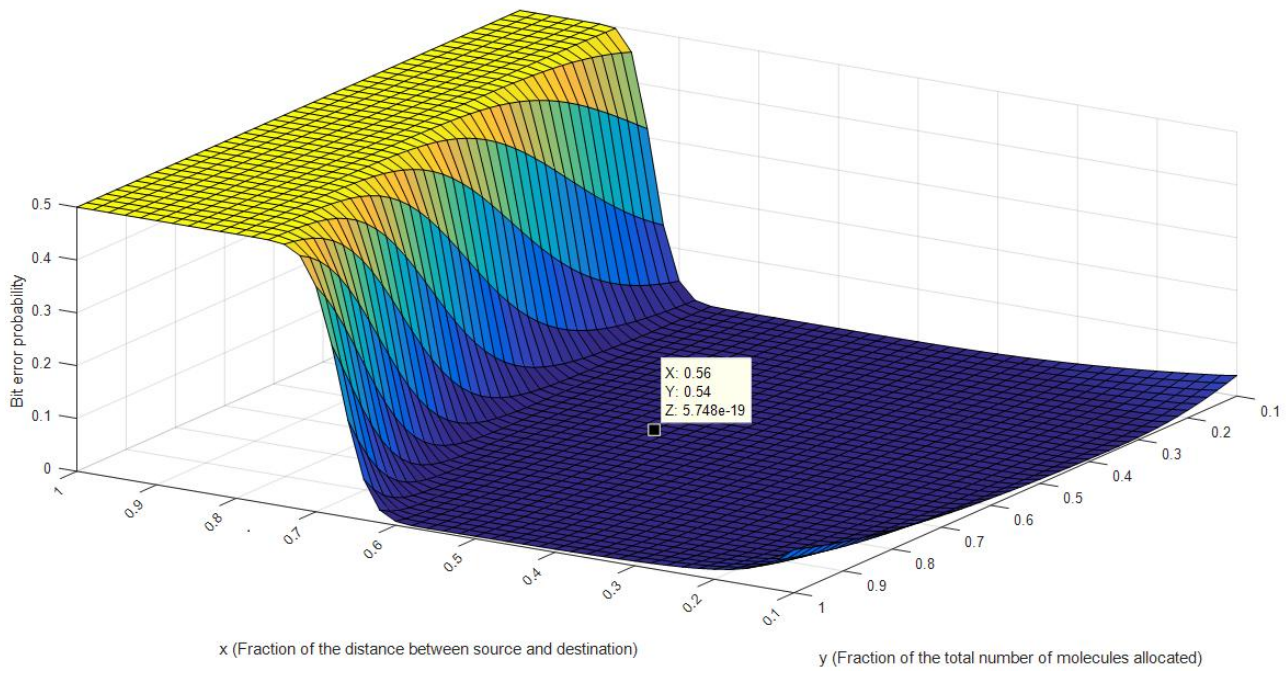


Fig. 3.2: 3D plot of bit error probability as a function of x (fraction of distance between source and destination) and y (fraction of total number of allocated molecules)

It can be seen from the 3D plot that the objective function is not convex. Further, it can be deduced from the plot that the minimum value of the bit error rate is 5.748 x 10^{-19} at x = 0.56 and y = 0.54. This can be predicted by the color code of the points on the graph. The lighter the color, the higher is the value of the function in this case P_e[k] and the darker the color, the lowest is the value of the function. The exact value at any point can be evaluated using the data cursor tool in MATLAB figure window.

Now since the problem is not convex, it needs to be first formulated into a convex joint optimization problem and then, by using any mathematical method to solve a convex problem, the solution to this problem can be deduced.

There are two ways in literature [2], [19] which can be used to make the above optimization problem a convex problem. One of the methods is to first obtain the second derivatives of the function with respect to the two variables x and y and then, apply constraints over the second derivatives such that the value of second derivatives become positive and the function becomes convex based on the constraints. This will ensure the convexity of the function in some regions based on the constraints. Once the convex optimization problem is formulated which will also include the constraints assumed to make the function convex, the solution to the convex problem can be obtained by using any mathematical method such as Karush-Kuhn-Tucker (KKT) conditions or any other method proposed in literature [20].

Chapter 4

Analysis of Performance based on System Parameters

In this chapter, the impact of different parameters is analyzed on the performance of the relay-assisted MC system. These parameters include molecular degradation coefficient, drift velocity, size of micromachines – source, relay and destination. The analysis is presented in the form of numerical results. Some numerical results are also shown for relay-assisted transmission in comparison with to direct transmission.

4.1 Significance of Relay Node on Error Probability based on Detection Threshold at Destination

- The error probability performance of the system as a function of the detection threshold for relay-assisted transmission, v = 0.3 mm/s, α = 54 s^{-1} , T = 5 ms and d_{SD} = 2 μm is presented in Fig. 4.1.
- The performance for direct transmission is also shown for comparison. In direct transmission, only node S-to-node D link with no intermediate relay node is assumed. Values assigned are N_A = N_B = 300 in the relay-assisted case and N_A = 600 in the direct transmission for a fair comparison.
- It is observed from Fig. 4.1 that relay node significantly improves the system performance in comparison with the direct transmission as the curve for relay-assisted transmission is much steeper than that for direct transmission. The minimum bit error rate for relay-assisted transmission is in the range of 10^{-14} while that for direct transmission is in the range of 10^{-3} approximately.

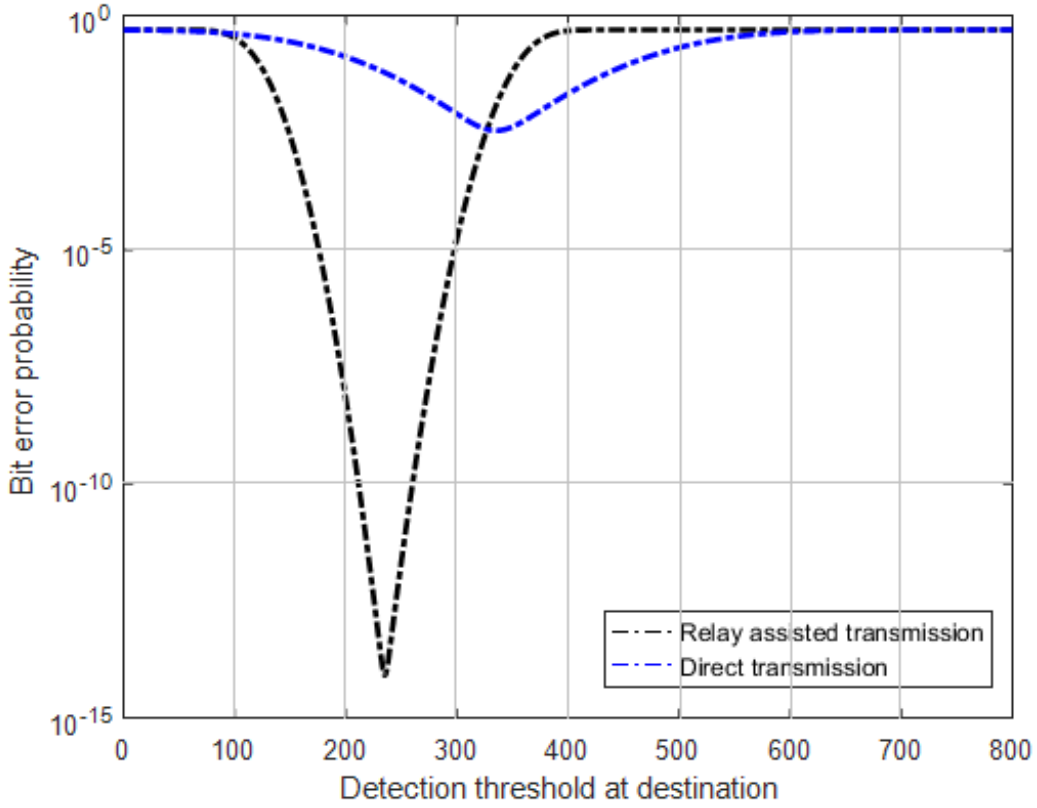


Fig. 4.1 Bit error probability as a function of detection threshold at destination for relay-assisted and direct transmission.

4.2 Significance of Relay Node on Error Probability based on Drift Velocity

- In Fig. 4.2, the impact of the value of drift velocity on the performance of the diffusion based MC system with and without the relay node is studied for T = 2 ms, α = 40, r_S=r_R=r_D=0.2 μm and d_{SD}= 1 μm. Values assigned are N_A = N_B = 300 in the relay-assisted case and N_A = 600 in the direct transmission for a fair comparison. In the relay-assisted transmission, the optimal detection threshold is used as the one derived using MATLAB function fminbnd.
- Fig. 4.2 demonstrates that increasing the value of drift velocity reduces the error probability non-linearly. The results show that when the drift velocity increases from v = 0.3 mm/s to v = 0.7 mm/s, the error probability decreases from 10^{-10} to 10^{-20} in the relay-assisted transmission, while in the direct transmission, the error probability decreases from 10^{-2} to 10^{-7}.

- For lower drift velocities up to 0.5 mm/s, change in error probability w.r.t to change in drift velocity in relay assisted transmission is greater than that for direct transmission. However, the performance improvement is observed with increasing the drift velocity in both cases and hence low error probabilities can be achieved. This is because increasing the drift velocity results in decreasing the ISI. In other words, as velocity increases, the released molecules get absorbed by the receiver with higher probability and hence the residue molecules from the previous symbol durations causing ISI decrease at the receiver.

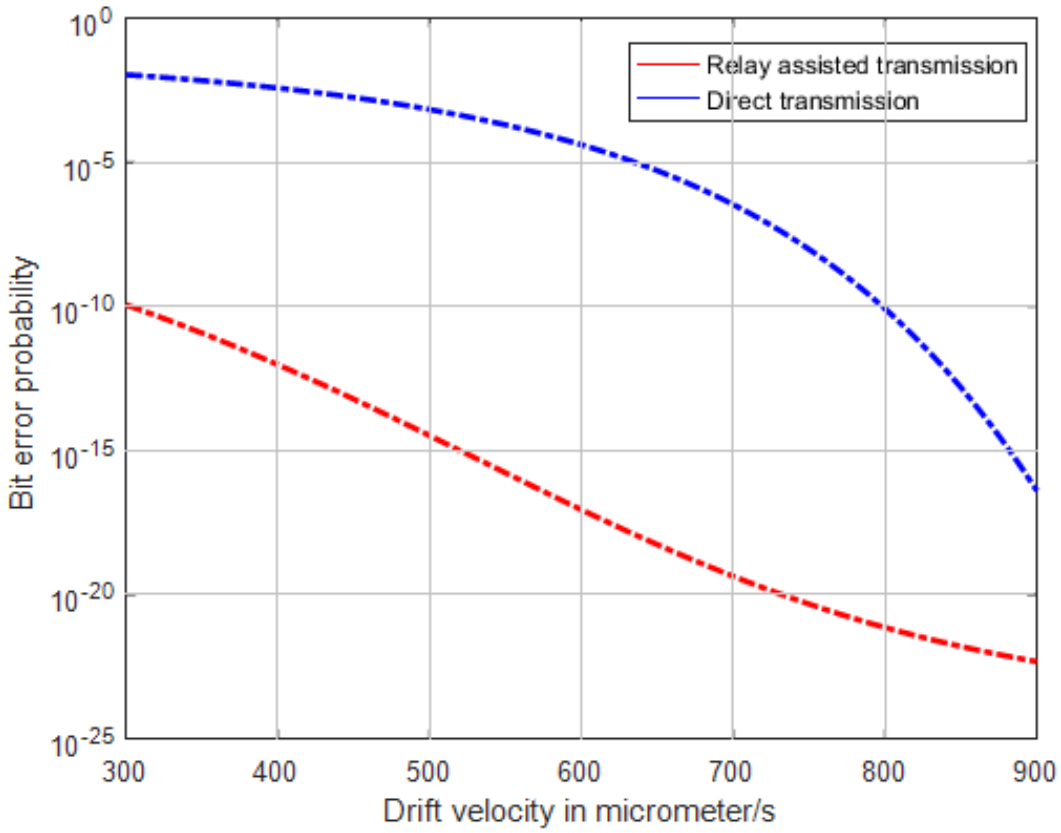


Fig. 4.2 Bit error probability as a function of drift velocity for relay-assisted and direct transmission.

4.3 Significance of Line Transmitter, Relay and Receiver

- To observe the effect of finite dimensions of transmitters and receivers, the radius of the source, relay and destination is varied according to the distance between any two micromachines i.e. source and relay i.e. $r_S = r_R = r_D = x * d_{sr}$ where $x \in (0, 0.5)$. The error probability is plotted as a function of x in Fig. 4.3 for different values of distance between source and

destination, T = 5 ms, v = 0.3 mm/s, α = 54 s^{-1}, and N_A=N_B=300. The radius of source, relay, and destination will be same at any instant as x varies and d_{SR}=d_{RD}=0.5d_{SD}.

- It is observed from Fig. 4.3 that as x tends to 0 that is the radius of the components (source, relay, and destination) become negligible and the components become point source, the error probability is maximum.
- On the other hand as x tends to 0.5 that is the radius of the components become comparable to the distance between two elements and the surface of the components touch each other, the error probability reduces because the effective distance between the surfaces of the transmitter and receiver reduces and molecules will be absorbed by the receiver in no time without getting affected by ISI, other noise sources or degradation.
- As observed in Fig. 4.3, with increase in the value of distance between source and destination, the curve shifts upwards i.e. the bit error probability increases.

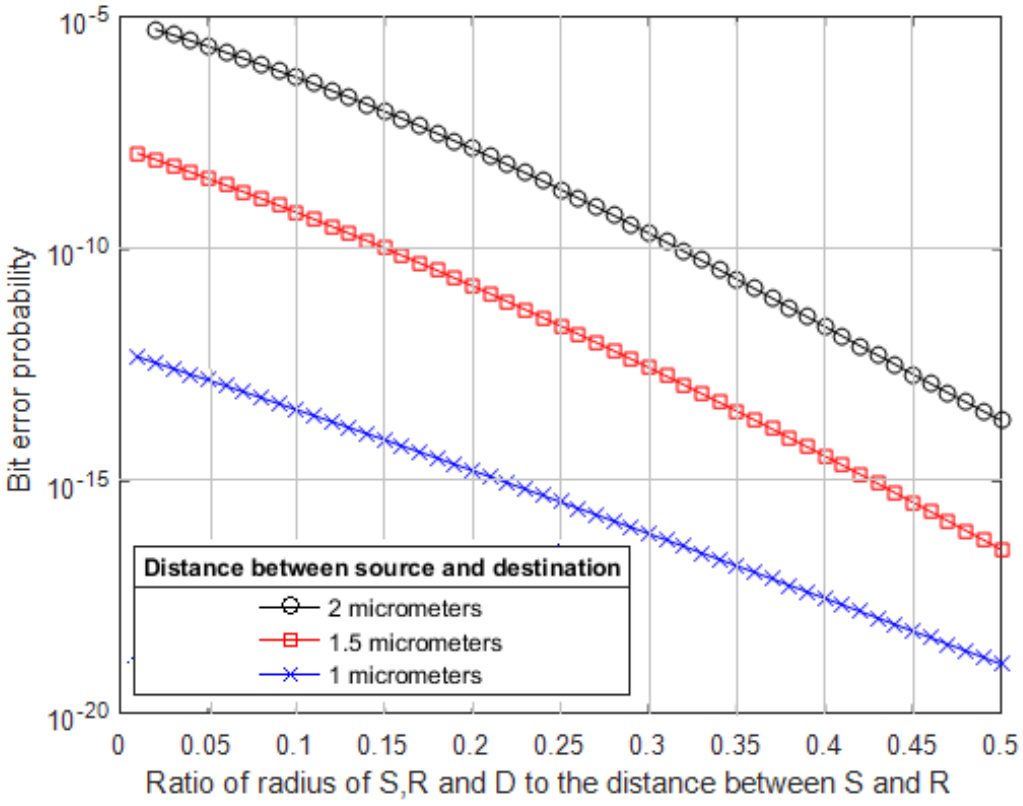


Fig. 4.3 Bit error probability as a function of fraction of d_SR for different values of distance between source and destination (d_{SD})

4.4 Effect of Molecular Degradation

- Fig. 4.4 demonstrates the impact of molecular degradation on the bit error probability for different values of symbol time duration, r_S=r_R=r_D=0.5 μm, v = 0.3 mm/s, d_{SD}=2 μm and N_A=N_B=400. The curve is plotted for α ϵ (1.4, 173) from half-life values $\lambda_{1/2}$ ϵ (0.004, 0.512) from literature [17].

- The observed effects from Fig. 4.4 match the observations in the literature [17]. The observations in literature [17] state that for short symbol durations, molecules having lower half-lives i.e. molecules that have larger degradation rates will provide better BER and thus, lesser performance impairment. While for longer symbol duration, molecules with greater half-lives i.e. molecules that will have lower degradation rates will provide better BER.

- Thus, it can be observed from Fig. 4.4 that for short time duration i.e. T = 0.005 s with increase in degradation coefficient, the BER is improved up to certain value of degradation coefficient after which with increase in degradation coefficient, the BER increases.

- In Fig. 4.4, comparison of the curves for T=0.01 and T=0.05 s show that for short time duration i.e. T=0.01 s, the change in error probability is greater than that for greater time duration.

- The above results are observed because for larger time duration and at smaller coefficient of degradation, $Pe|0$ (the probability with which the bit 0 sent from the source will be inaccurately detected as 1) is more significant contributor to the overall error since molecular communication systems suffer from ISI significantly. However, for short time duration, this effect is not much significantly observed. On the other hand, for short time durations and at higher degradation coefficient, the molecules get destroyed so fast that they cannot deliver the encoded information to the receiver. This is, however, not significant in larger time durations at larger degradation coefficient since the molecules get enough time to reach the receiver before getting degraded.

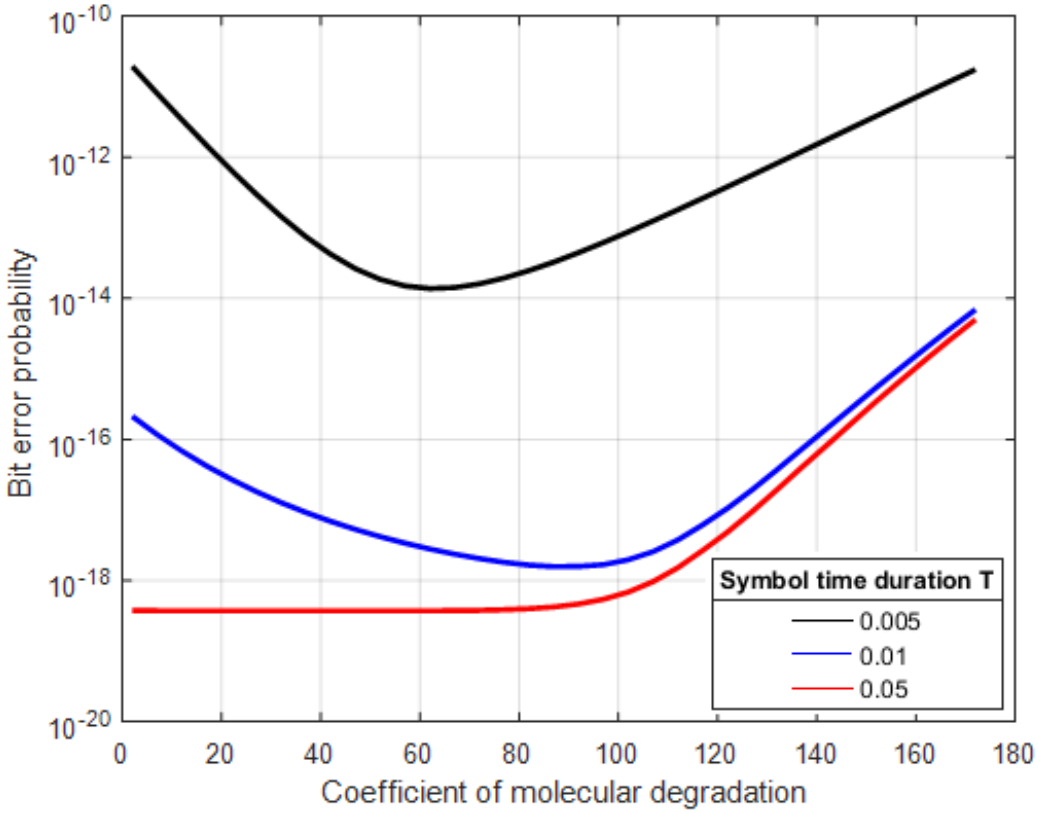


Fig. 4.4 Bit error probability as a function of coefficient of molecular degradation for different values of symbol duration.

Chapter 5

Conclusion and Future Scope

In this report, the error performance of the relay-assisted diffusion-based MC system with linear transmitter is evaluated. A closed-form expression for the bit error probability based on the normal approximation to the distribution of the number of received molecules is derived. Furthermore, an optimization problem to minimize the derived error probability is formulated with the optimization variable being the detection threshold at destination and a solution using MATLAB's optimization toolbox is proposed which give nearly the same optimal values as observed in the numerical results. The joint optimization problem is just introduced in this report while a solution to the problem is not proposed. Ultimately, investigation is done on how the system parameters such as drift velocity, position of the relay from the source, molecular degradation, volume of micromachines and the number of allocated molecules affect the performance of the system. Numerical evaluation revealed that with increase in the size of the components or micromachines with respect to distance between the components, the error probability is reduces. Moreover, with a constant molecular budget, the relay-assisted transmission model achieves better performance than the direct transmission model. In addition, for lower drift velocity, performance degradation is significantly reduced for relay-assisted MC model.

The future scope of this project will be to use another method to optimize the threshold value to obtain results as close to the observed results. Another future work will be to find a solution to the joint optimization problem introduced in chapter 2. In addition, the numerical analysis will be done by assigning practical values relevant to a particular application to system parameters.

Appendices

Appendix A

Error Function

The Gauss error function or the error function is a special function (non-elementary), in mathematics, of sigmoid shape that occurs in probability, statistics, and partial differential equations describing diffusion. It is defined as:

$$erf\left(x\right)=\frac{1}{\sqrt{\pi}}\int_{-x}^{x}\exp\left(-t^2\right)dt$$

$$\therefore erf\left(x\right)=\frac{2}{\sqrt{\pi}}\int_{0}^{x}\exp\left(-t^2\right)dt$$

The plot for the error function is presented in Fig. A.1. In statistics, for nonnegative values of x, the error function has the following interpretation: for a random variable X that is normally distributed with mean 0 and variance ½, erf(x) describes the probability of X falling in the range [−x, x].

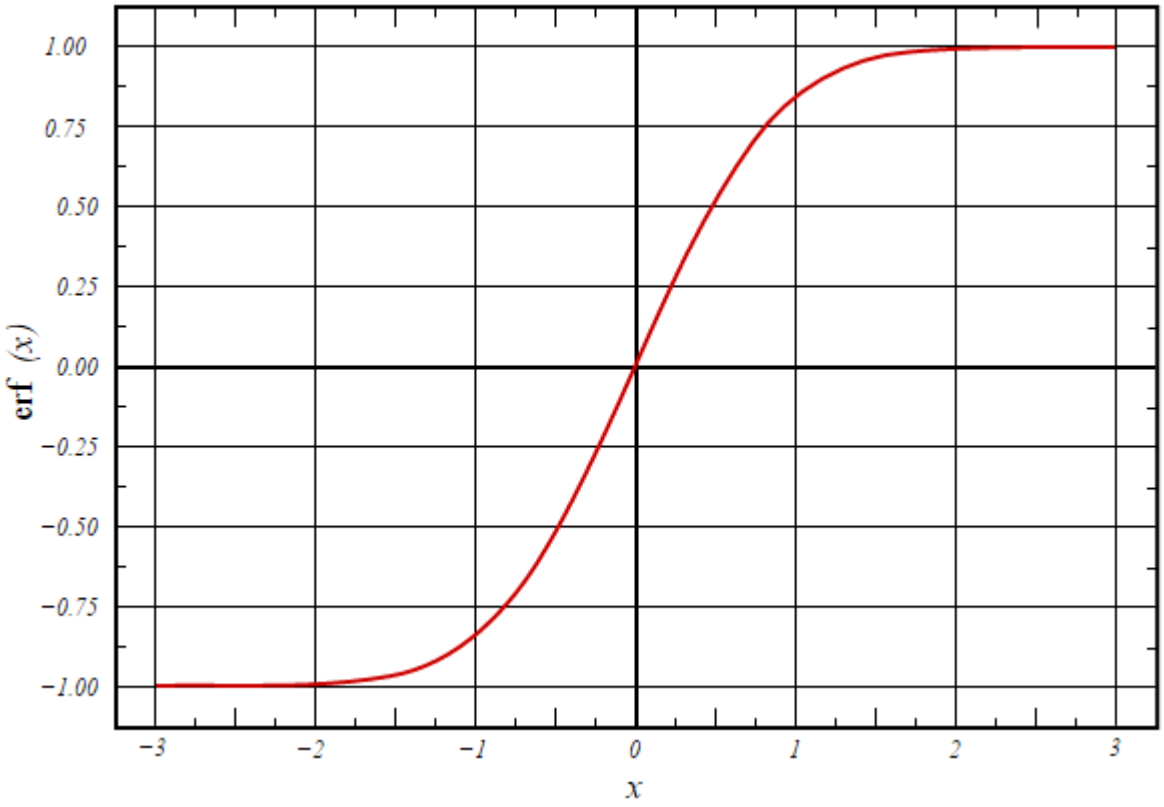


Fig. A.1: Plot of erf(x).

The complementary error function (erfc), is defined in terms of error function as

$$erfc(x) = 1 - erf(x)$$
$$\therefore erfc(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} \exp\left(-t^2\right) dt$$

Derivative Properties:

The derivative of the error function is given as:

$$\frac{d}{dx} erf\left(x\right) = \frac{2}{\sqrt{\pi}} \exp\left(-x^2\right)$$

Related functions:

Q-function: The Q-function is the tail probability of the standard normal distribution $\phi\left(x\right)$.

In other words, Q(x) is the probability that a normal (Gaussian) random variable will obtain a value larger than x standard deviations above the mean.

If the underlying random variable is y, then the proper argument to the tail probability is derived as:

$$x = \frac{y - \mu}{\sigma}$$

where μ is the mean and σ is the standard deviation.

This x expresses the number of standard deviations away from the mean.

The Q-function is defined as:

$$Q\left(x\right) = \frac{1}{\sqrt{2\pi}} \int_{x}^{\infty} \exp\left(-\frac{t^2}{2}\right) dt$$
$$Q\left(x\right) = 1 - Q\left(-x\right)$$

The Q-function can be expressed in the form of error function as:

$$Q\left(x\right) = \frac{1}{2}\left(\frac{2}{\sqrt{\pi}} \int_{x/\sqrt{2}}^{\infty} \exp\left(-t^2\right) dt\right)$$
$$\therefore Q\left(x\right) = \frac{1}{2} - \frac{1}{2} erf\left(\frac{x}{\sqrt{2}}\right)$$
$$\therefore Q\left(x\right) = \frac{1}{2} erfc\left(\frac{x}{\sqrt{2}}\right)$$

Appendix B

Quasiconvex Function

In mathematics, a quasiconvex function is a real-valued function defined on an interval or on a convex subset of a real vector space such that the inverse image of any set of the form (∞, a) is a convex set. Informally, along any stretch of the curve the highest point is one of the endpoints. The negative of a quasiconvex function is said to be quasiconcave. All convex functions are also quasiconvex, but not all quasiconvex functions are convex, so quasiconvexity is a generalization of convexity.

A function $f : S \to \mathbb{R}$ defined on a convex subset S of a real vector space is quasiconvex if for all $x, y \in S$ and $\lambda \in [0,1]$ we have

$$f\left(\lambda x + (1-\lambda) y\right) \leq \max\left\{ f(x), f(y) \right\}$$

In words, if f is such that it is always true that a point directly between two other points does not give a higher value of the function than both of the other points do, then f is quasiconvex.

Appendix C

Apriori Probabilities for Bits Transmitted from Relay

The probability with which the relay will detect bit 0 or bit 1 will be the apriori probability of bit 0 and bit 1 for the diffusion process between relay and destination in the $(k+1)^{th}$ slot.

Let x_R denote the bit detected by the relay at the end of the k^{th} slot and x_S denote the bit sent from the source at the start of the k^{th} slot.

Then, the apriori probability b_1 will be given as:

$$b_1 = \Pr(x_s = 0).\Pr(x_R = 1 | x_S = 0) + \Pr(x_s = 1).\Pr(x_R = 1 | x_S = 1)$$

where $\Pr(x_R = 1 | x_S = 0) = \Pr(Q_A > \tau_R | x_S = 0)$ and $\Pr(x_R = 1 | x_S = 1) = \Pr(Q_A > \tau_R | x_S = 1)$

$$\Pr(Q_A > \tau_R | x_S = 0) = Q\left(\frac{\tau_R - \mu_{A0}}{\sigma_{A0}}\right)$$

$$\therefore \Pr(Q_A > \tau_R | x_S = 0) = \frac{1}{2}\left(1 - erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}}\right)\right)$$

Similarly,

$$\Pr(Q_A > \tau_R | x_S = 1) = Q\left(\frac{\tau_R - \mu_{A1}}{\sigma_{A1}}\right)$$

$$\therefore \Pr(Q_A > \tau_R | x_S = 1) = \frac{1}{2}\left(1 - erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}}\right)\right)$$

$$\Pr(x_S = 0) = \Pr(x_R = 1) = \frac{1}{2}$$

$$\therefore b_1 = \frac{1}{2}.\left[\frac{1}{2}\left(1 - erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}}\right)\right) + \frac{1}{2}.\left(1 - erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}}\right)\right)\right]$$

$$\therefore b_1 = \frac{1}{2} - \frac{1}{4}\left[erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) + erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) \right]$$

Similarly, the apriori probability will be given as:

$$b_0 = \Pr(x_s = 0).\Pr(x_R = 0 \mid x_S = 0) + \Pr(x_s = 1).\Pr(x_R = 0 \mid x_S = 1)$$

Where $\Pr(x_R = 0 \mid x_S = 0) = \Pr(Q_A < \tau_R \mid x_S = 0)$ and $\Pr(x_R = 0 \mid x_S = 1) = \Pr(Q_A < \tau_R \mid x_S = 1)$

$$\Pr(Q_A < \tau_R \mid x_S = 0) = 1 - Q\left(\frac{\tau_R - \mu_{A0}}{\sigma_{A0}} \right)$$

$$\therefore \Pr(Q_A < \tau_R \mid x_S = 0) = \frac{1}{2}\left(1 + erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) \right)$$

Similarly,

$$\Pr(Q_A < \tau_R \mid x_S = 1) = 1 - Q\left(\frac{\tau_R - \mu_{A1}}{\sigma_{A1}} \right)$$

$$\therefore \Pr(Q_A < \tau_R \mid x_S = 1) = \frac{1}{2}\left(1 + erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) \right)$$

$$\therefore b_0 = \frac{1}{2}.\left[\frac{1}{2}\left(1 + erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) \right) + \frac{1}{2}.\left(1 + erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) \right) \right]$$

$$\therefore b_0 = \frac{1}{2} + \frac{1}{4}\left[erf\left(\frac{\tau_R - \mu_{A0}}{\sqrt{2\sigma_{A0}^2}} \right) + erf\left(\frac{\tau_R - \mu_{A1}}{\sqrt{2\sigma_{A1}^2}} \right) \right]$$

Sources of Figures:

Fig. 1.1 – Literature [1]

Fig. 1.2 – Internet

Fig. A.1 – Wikipedia

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